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TECHNICAL ABSTRACTS

LASER BASED MULTI-PARAMETER MEASUREMENTS IN DENSE AUTOMOTIVE DIRECT INJECTION SPRAYS

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It is demonstrated in this work that multiple scalar and vector quantities can be measured in dense sprays from automotive swirl injectors by advanced laser diagnostic techniques. Such injectors are currently being developed for gasoline direct injection engines. Measurements are generally difficult in these dense sprays using conventional techniques, such as Phase Doppler Anemometry and Particle Image Velocimetry, because of the high number densities of droplets, the optical thickness of the medium and multiple light scattering effects. Thus, we developed a number of new measurement techniques to overcome these problems. Specifically, we did 2-D velocity measurements by laser-based flow tagging, 1-D droplet temperature measurements by spontaneous Raman scattering, and 1-D droplet diameter measurements by Raman/Mie combination. Initial measurements have been done in swirling sprays provided by Volkswagen AG, Wolfsburg, and Robert Bosch GmbH, Stuttgart, Germany. Velocity measurements by laser based flow tagging is performed as follows: The gas (or liquid) phase is tagged on a number of tag lines (‘write' laser grid) by inducing either photodissociation or phosphorescence. The tracer molecules are convected with the flow and probed after a certain delay. The instantaneous velocity field is determined from the two images by time-of-flight analysis using an optical flow algorithm.

The temperature measurement technique is based on the shape and spectral position of the OH stretching Raman scattering band, which can be recorded in alcohol sprays. The accuracy achieved in this way is about ±2 °C. These measurements are performed by using a spatially resolving optical multichannel analyzer as the detector. Thus, several other vibrational Raman lines and elastic scattering can be recorded simultaneously. This yields the possibility to obtain additional spatially resolved information, for example, air/fuel ratio, vapor/liquid mass fraction, or gas temperature simultaneously. In particular, it is demonstrated that the Sauter mean diameter can be measured in dense evaporating alcohol sprays by exploiting Mie scattering and the Raman scattering line from the liquid phase.

Ignition Time Correlations for n-Heptane/O_2/Ar Mixtures: A Parametric Study of Experimental Data and Kinetic Modeling

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Ignition time measurements of *n*-heptane/O_2/Ar mixtures have been studied behind reflected shock waves over the temperature range of 1300-1700 K and pressure range of 1-6 atm; the mixture composition was varied from 0.2-1.8% *n*-heptane, with an equivalence ratio of 0.5-2.0. To more precisely determine the fuel mole fraction of the test mixture, a new technique has been employed in place of the more traditional manometric method. This technique utilizes a 3.39 μm HeNe laser and multiple-pass set-up to measure in-situ laser absorption of the fuel, resulting in a reduction of the fuel mole fraction uncertainty. The ignition time was defined as the time interval between the arrival and reflection of the incident shock at the endwall and the rapid rise of the CH emission signal recorded at that location. Sidewall pressure and CH emission traces were also recorded to more accurately model the combustion wave behavior behind the reflected shock.

The combustion chemistry is simulated using three detailed kinetic mechanisms: Held et al. (1997), Lindstedt and Maurice (1995), and Curan et al. (1998). A parametric study, conducted with all three models and the experimental data, suggests correlating the ignition time as a function of the equivalence ratio, oxygen mole fraction, and reflected pressure and temperature. The experimental data are correlated as follows:

$$\tau(s) = 4.50\times10^{-12} X_{O2}^{-0.63} \phi^{0.85} P^{-0.55} \exp(46{,}000/RT)$$

where X_{O2} is the oxygen mol fraction, ϕ is the equivalence ratio, P is the total pressure in atm, and the activation energy is expressed in cal/mol. To enable comparison to the other work, the data for the present study have also been correlated in the more traditional form:

$$\tau(s) = 4.37\times10^{-14}\, [n\text{-heptane}]^{0.84} [O_2]^{-1.42} \exp(46{,}400/RT)$$

where the concentration of fuel and oxygen are expressed as moles/cm^3.

The kinetic models of Lindstedt and Maurice, and Curran et al. were found to reasonably predict the present ignition time measurements; the model of Held et al. was found to overpredict a majority of the current data. All three models closely predict the experimentally determined pressure dependence, but only the model of Curan et al. closely predicted the experimentally determined temperature dependence. Furthermore, the models of Lindstedt and Maurice and Curran et al. predict nominally the same oxygen mole fraction and equivalence ratio scaling as found experimentally.

The current data compares well in absolute magnitude with the previous shock tube work of Burcat et al. (1981), Vermeer et al. (1972) and Colket and Spadacinni (1999). It predicts an activation energy essentially identical to that of Vermeer et al., 15% higher than Colket and Spadacinni, and nominally 30% higher than that found by Burcat et al. The pressure dependence of the current study (n= -0.55) falls between the values determined by Burcat et al. (-0.3) and Vermeer et al. (-0.86) and Colket and Spadacinni (-0.8).

Decane Oxidation in a Shock Tube

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Normal Decane, $C_{10}H_{22}$, is one of the most obvious ingredients of diesel fuel. It was also defined as one of three ingredients (the others being methyl naphthalene and normal heptane) that their blend should be used to simulate diesel fuel. Since there are experimental results for simulating gasoline and kerosene combustion, the attention is now devoted to diesel fuel. The oxidation of decane is investigated by measuring the ignition delay of *n*-decane oxygen argon blends, in a single pulse shock tube. Due to the low vapor pressure of *n*-decane, the shock tube had to be heated to 100 °C in order to increase its concentration in the gas phase. Mixtures of 0.5 to 1.5% decane, and 2.3 to 4.2% oxygen diluted in argon, were used at pressures between 1.8 to 9.4 atm.

The overall ignition delay of decane based on a s=2 spread of 144 experiments is:

$$\tau(s) = 10(\pm0.2)^{-12}\exp(+34{,}240/RT)\ [C_{10}H_{22}]^{0.60\pm0.06}[O_2]^{-1.30\pm0.04}[Ar]^{0.08\pm0.05}$$

The overall ignition delay of decane based on a s=3 spread of 168 experiments is:

$$\tau(s) = 10(\pm0.4)^{-11.9}\exp(+34{,}600/RT)\ [C_{10}H_{22}]^{0.66\pm0.09}[O_2]^{-1.33\pm0.06}[Ar]^{0.06\pm0.07}$$

Post shock and preignition samples of gas were gathered and analyzed for products in a gas chromatograph. The post shock products detected were: CO_2, CH_4, C_2H_4, C_2H_6, C_3H_6, C_4H_6, 1-C_4H_8, 1-C_5H_{10}, 1-C_6H_{12}, 1-C_7H_{14} and 1-C_8H_{16}. No higher products than C_8 were detected except for decane itself. Kinetic modeling is being performed and the results for the lower hydrocarbons up to hexane are satisfactory. The research is being continued.

Effects of a Uniform Magnetic Field on the Combustion and Emission Characteristics of Premixed Laminar Flames

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The effects of an electric field on a flame or combustion process has almost been elucidated regardless of the field property; either uniform or nonuniform, steady or unsteady. The direct effects of a magnetic field, however, are not known yet, although some indirect effects of a nonuniform magnetic field have been reported by several investigators. We tackled this problem using a super-conducting magnet and encountered considerable difficulties as follows. (1) The indirect effects easily surpassed the direct ones because no magnetic field uniform enough was attainable if we used a magnetic coil. This fact restricted the precision of experimental data in spite of our effort. (2) Optical and intrusive measurements were very difficult because the object flame was located in a long and slender nontransparent vertical tube of 51 mm i.d. and 500 mm long.

The magnetic flux density falls by a few percent from the axis to the tube wall. Oxygen, a gas having rather strong magnetism, on the other hand, is consumed in the flame zone and produces a concentration gradient in the radial direction. Both gradients interact with each other and generate an inward secondary flow. This secondary flow accelerates the central stream upwards and decelerates the peripheral one.

A Bunsen type propane/air premixed laminar flame was formed within the vertical tube placed at the center of a super-conducting magnet generating a nearly-uniform upward magnetic field of 5 T. It was observed how the magnetic field affected the flame stability limit equivalence ratio, flame contour, burning velocity and the distribution patterns of gasification temperature and nitrogen oxides (NO and NO_2) concentration in and around the flame. It was found that the temperature and burning velocity of a flame, which were dominated by high-speed chemical reactions, were not affected by a magnetic field as intense as 5 T within the precision of the present experiment. Meanwhile, it appeared that the magnetic field had a slight retardation effect on the process of nitrogen oxide formation dominated by low-speed chemical reactions. If, however, the above-mentioned acceleration of the central stream by the secondary flow were taken into account, this apparent retardation effect should significantly be discounted, because the flow acceleration should result in a reduced reaction period until reaching a fixed point around the axis.

Burning Velocity Measurements and Calculations of Methane/Propane Mixtures

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In this work, measurements of the adiabatic burning velocity in a flat flame are presented. The burner used in this work provides a flat, stretchless flame, which is effectively made adiabatic. This is achieved by tuning the stabilizing heat loss of the flame to compensate for the heat gain from the unburnt gases as they pass the burner plate. The heat flux balance is monitored by measuring the temperature distribution of the burner plate with thermocouples.

Methane/propane mixtures are investigated in various compositions, ranging from pure methane to pure propane, with an equivalence ratio from 0.6 to 1.4. To compare the experimental results with numerical simulations, calculations are performed; one set of calculations is carried out using the GRI 2.11 reaction mechanism. Another set is carried out with a Warnatz mechanism, which includes a C4 chain. To be able to use the GRI 2.11 mechanism for propane flames, it has been extended with the C3 branch of the Warnatz mechanism. The flames are calculated as free flames, without interaction to the burner.

The results show that there is good agreement for the measured methane burning velocities with the calculations based on the GRI 2.11 mechanism. However, the calculations based on the Warnatz mechanism appear to be significantly higher, up to 5 cm/s. For propane, both simulations show higher burning velocities than the measurement results.

For methane/propane mixtures, both GRI 2.11 and Warnatz based calculations show the same tendency: the propane content increases the burning velocity. The influence is considerably larger in mixtures having a methane fraction above 50%, as compared to mixtures approaching 100% propane. The same tendency is seen in the measurements.

ION MOLECULE CHEMISTRY AT TEMPERATURES UP TO 1800 K

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While most ion molecule chemistry has been measured at or near room temperature and below, high temperature plasmas occur in the ionosphere, combustion, plasma reactors, and plasmas associated with atmospheric reentry and hypersonic flight. For these reasons, we have developed a flowing afterglow capable of measuring both rate constants and branching ratios at temperatures up to 1800 K. Additional information can be obtained from the temperature dependence data by comparing the high temperature data to drift tube data. This yields information on how internal energy affects reactivity. We have found rotational and translational energy often control reactivity similarly and that vibrational energy often has a more pronounced influence on reactivity than does translational energy or rotational energy. A good example is the reaction of O_2^+ with CH_4. The rate constant for this reaction increases dramatically at high temperature and 50% of the products are not observed at low temperature or elevated translation energy showing that CH_4 vibrational excitation enhances overall reactivity in part by opening new channels, i.e. state specific chemistry. Even in larger systems we have found that internal and translational energy behave differently. For example, we have observed in the charge transfer reactions of NO^+ and O_2^+ with alkylbenzenes that electronic and internal energy is more efficient at promoting dissociation than is translational energy. This chemistry along with other representative examples will be presented.

NEW INSTRUMENT FOR MEASURING ION-MOLECULE KINETICS AT ELEVATED PRESSURES: THE TURBULENT ION FLOW TUBE

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Ion molecule kinetics have traditionally been measured at pressures of 10 torr or less with a few exceptions. The few studies at high pressure have found interesting new processes. We present the first data taken on a new instrument for studying ion kinetics at pressures from 20-750 torr. The turbulent ion flow tube is based on the similar neutral apparatus from Seeley and Molina. Ions are created upstream from a radioactive ion source. A fast flow of carrier gas transports the ions downstream and measurements are made in the normal manner for a flow tube experiment. An upgrade in progress will allow temperature variability and operation at pressures up to 2 atm. The first system studied was the reaction of SF_6^- with SO_2. The rate constant was rapid and constant throughout the pressure range and three products were formed, SF_5^-, FSO_2^- and $F_2SO_2^-$. Within uncertainty, the branching ratio was also independent of pressure. The reactions of SF_6^- with three solvent molecules, H_2O, CH_3OH, and C_2H_5OH, were also studied. These reactions are considerably more complex. The decline in the SF_6^- signal is second order in the concentration of reactant. In all cases, the reaction proceeds through a cluster ion between SF_6 and the solvent, $SF_6^-(X)$. The equilibrium measurements indicate a $-\Delta G = 4\text{-}5$ kcal/mole. $SF_6^-(X)$ in turn reacts with another solvent molecule producing two product ions. The rate for this process is slow, with rate constants on the order of 10^{-14} $cm^3\ s^{-1}$. In the H_2O reaction, SF_4O^- and $F^-(HF)_2$ were formed. In the alcohol reactions $F^-(HF)$ and $F^-(HF)_2$ were formed. The product ions are further solvated by the reactant neutral. Slow solvent switching of the second HF in $F^-(HF)_2$ is also observed with the alcohols.

A New Method to Minimize High Temperature Corrosion Resulting from Alkali Sulfate and Chloride Flame Deposition

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Based on an earlier understanding of the parameters that control flame generated deposition of Na_2SO_4 or NaCl onto cooled surfaces immersed in a flame, a new process† has been developed to inhibit their formation. It is seen that no alkali sulfate is formed if tungsten salts are added to a flame containing an alkali (sodium or potassium), sulfur and chlorine, when the tungsten-to-alkali ratio is larger than about 2-fold on an atomic basis for sodium and possibly a little higher (4-fold) for potassium. Instead, the alkali exhibits a greater affinity for the tungsten and benign alkali tungstates are deposited. This is further confirmed in experiments in which an Na_2SO_4 deposit is initially formed on a probe and then is seen to be fully converted by the addition of sufficient tungsten and overlaid by a similar tungstate growth. Deposition appears to closely reflect the relative thermodynamic stabilities of these salts and follows the order $Na_2WO_4 > Na_2SO_4 > NaCl > Na_2CO_3$. Conversions can occur in the direction of greater stability but are irreversible. The method appears to be insensitive to fuel, equivalence ratio or general flame parameters. Deposits have been acquired on stainless steel and platinum clad probes operating in the temperature range 600 to 900 K. Analysis has utilized Fourier transform Raman spectroscopy and Inductively Coupled Plasma Atomic Emission. An analysis also has been completed of other potential additives that might act similarly in preferentially binding the alkali. Indicates are that only niobium and tantalum are possibilities but are not as attractive commercially. A preliminary examination of potential interferences has been made. This concerns whether any other element might have a greater affinity for the tungsten over that of the alkali. Calcium, strontium and barium appeared to fall in this potential category having well defined tungstates. However, thermodynamic calculations and preliminary experiments indicate that these still favor sulfate formation and do not tie up any of the available tungsten in the system.

This process has been patented with the U.S. Patent Office, Serial No. 09/505,007, February 15, 2000, University of California, Oakland, CA.

PAHs Formation in Premixed Flames of Gaseous Fuels: An Experimental Study

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Polycyclic aromatic hydrocarbons (PAHs) belong to the most toxic substances emitted to the atmosphere from anthropogenic sources. The exact mechanisms of formation of this group of compounds are not well understood. The goal of the experimental measurements was to determine the axial concentrations of selected PAHs in laboratory scale atmospheric pressure methane/air and methane/toluene/air flames for various fuel/air ratios. In order to examine the influence of acetylene on PAHs formation the fuel was doped with acetylene.

The experimental setup consists of three basic components – a mixture preparation system, a ceramic combustion chamber with movable burner and a sampling system. Air-fuel mixture preparation system consists of flow rotameters, reducing valves, mixer and transfer lines. Toluene was evaporated and mixed with air. After combining the flows of CH_4, C_2H_2 C_7H_8 and air they were passed through a long line to ensure good mixing. In order to obtain axial profiles of PAHs concentrations the burner was moved relative to the stationary probe. Samples were obtained using a stainless steel water cooled probe. PAHs were caught on an XAD-2 trap. Samples were extracted using a Soxhlet apparatus. Final separation, detection and identification was realized by means of gas chromatography combined with a flame ionization detector (GC-FID). The flame temperatures were measured by using PtRh10%-Pt thermocouple.

The selected PAHs axial concentration profiles and temperatures were measured in an atmospheric pressure premixed CH_4/air and CH_4/C_7H_8/air flames at the fuel equivalence ratios: ϕ=0.9-1.1. The methane flow rate was about 0.12 m_n^3/h. In the case of CH_4/C_7H_8/air flame the toluene mol fraction was 7% of the gas flow (about 25% of the thermal output). The methane was doped with toluene in order to evaluate the influence of the presence of aromatic structure on formation and emission of PAHs. Moreover, the measurements of selected PAHs concentrations at the distance of 100 mm from burner mouth as a function of fuel/air ratio were performed. Gas/air mixture flow velocity in all cases was at the level of 23 cm/s.

The axial concentrations profiles of selected PAHs in studied flames indicated that PAHs are formed rapidly at the beginning of the flame, then their concentrations decrease. In some cases concentration of selected PAHs further increase downstream. The final PAHs concentrations in CH_4 flames doped with toluene (aromatic structure) are higher than those in CH_4 flames especially at ϕ>1.1 (rich mixture). Also addition of acetylene produces much higher PAHs concentrations - it confirms the significant role of acetylene in the processes of PAHs formation.

The effect of the fuel/air ratio on the final concentrations of PAHs in both (CH_4/air and CH_4/C_7H_8/air) flames was studied as well. The PAHs reach their minimum concentrations at ϕ=1.05 and their concentrations increase with increasing or decreasing of ϕ. This dependence is a result of flame temperature, local oxygen concentration and residence time.

Further investigations of the influence of other parameters of the combustion process (fuel and oxidizer composition, excess air ratio) on PAHs concentrations profiles are planned. The semiempirical model of PAHs formation and destruction will be constructed on the basis of the experimental measurements. The model will permit an evaluation of the levels of emissions of PAHs from gas-fired combustion devices.

Pesticide Waste Incineration in the Wet Process Cement Kiln

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Pesticide wastes (agricultural chemicals which exceeded a prescribed time limit) that have been accumulated underground in concrete graveyards or bunkers, now present a significant problem in Poland. They are scattered around the whole country. Their progressive unsealing poses a significant health risk to people due to groundwater, soil and air pollution. Incineration in professional hazardous waste incineration plants is one of methods used for disposal of pesticide wastes. There are not many incineration plants in Poland as compared to working cement plants whose number amounts to 18. Most of them are interested in utilization of various wastes (for example in the capacity of alternative fuels) in the process connected with the cement clinker production in rotary kilns. High temperatures existing in cement kilns(1370-1450 °C in the burning zone) as well as long gas-residence time (5-10 s) provide potentially excellent destruction conditions of wastes including hazardous wastes. According to the analysis of thermodynamic and technological conditions, the wet process kiln is best suited for the purpose.

The method of pesticide waste wet process cement kiln incineration has been worked out that allows to select such conditions for the process that do not have negative impact on the level of the air pollution, the quality of clinker and technological facilities durability. Analysis of most agricultural chemicals used in the past taking into consideration the type and the quantity of biologically active chemicals in these preparations, indicate that various pesticide wastes can include, for instance, up to 50% Cl, 80% S, 30% Cu, 15% Zn and 2.5% Hg (by weight). Copper and zinc are almost completely retained in the solid phase and built into the clinker like other probable components of the wastes that are neutral to the process (for example, Ca, Na, Mn and P). Chlorine and sulfur given off from the wastes in the form of HCl and SO_2 are absorbed by alkaline solid phase (CaO, Na_2O and K_2O) resulting in chlorides, sulfates or sulfites, and the efficiency of the reactions considerably increase outside the kiln (in lower temperatures). The major problem is caused by mercury vapors that can only partly condense on the fly ash surface and can be removed from flue gas with the aid of a dust collector.

According to analyses carried out for a standard wet process kiln, the most crucial parameters for the method are doses of Cl (for the sake of the process course and cement quality) and Hg (for the sake of emission to the air). Total chlorine input cannot exceed 0.16% with reference to the clinker mass. In most cases quantity of mercury inserted into the kiln (safe for air quality round the kiln chimney) cannot exceed 0.5-1.0 kg/h and should be divided into single doses as small as possible.

The analysis of possibility of pesticide waste thermal utilization in cement rotary kiln furnace were carried out for about 200 different kinds of pesticides collected in graveyard. For some pesticides it was possible to determine chemical constitution and their combustion enthalpy. For the other ones combustion enthalpy has been assumed by comparison to similar compounds. Thus, it was estimated that agriculture pesticide wastes can be treated as fuel with average calorific value about 2500 kJ/kg.

A Possible New Route Forming NO via N_2H_3

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A possible new route for NO formation in hydrogen combustion is explored. It is suggested that nitric oxide can be produced from N_2 via N_2H_3 in rich hydrogen/air mixtures at relatively low temperatures when other routes of NO formation are suppressed. The reaction sequence that converts molecular nitrogen into nitrogen oxides starts by the formation of NNH radicals

$$N_2 + H = NNH \quad (1)$$

$$N_2 + H + M = NNH + M \quad (2)$$

Fast recombination of the NNH radicals with H atoms leads to the formation of N_2H_2

$$NNH + H + M = N_2H_2 + M \quad (3)$$

and subsequently to the formation of N_2H_3

$$N_2H_2 + H + M = N_2H_3 + M \quad (4).$$

N-N bond cleavage occurs in the reaction of N_2H_3 with H_2 forming NH_3 and NH_2

$$N_2H_3 + H_2 = NH_3 + NH_2 \quad (5)$$

thus this possible new mechanism of the NO formation is identified as N_2H_3-route. NH_3 and NH_2 are oxidized mainly in the sequence $NH_3 \rightarrow NH_2 \rightarrow NH \rightarrow N \rightarrow NO$.

To clarify a role of the new possible route forming NO via N_2H_3, the combustion of hydrogen and air mixtures in well-stirred reactors is modeled employing an updated detailed H/N/O reaction mechanism or the same mechanism, but without N_2H_3 pathway. The detailed H/N/O mechanism used in the present study consists of 238 reversible reactions among 31 species. To suppress the N_2H_3-route of NO formation the rate constant of the recombination reaction (4) has been set to zero. The formation of nitric oxide is calculated and analyzed as a function of the mixture temperature, residence time, stoichiometry, and pressure in the reactor.

Key reactions of the N_2H_3 formation and consumption as well as other important reactions revealed by sensitivity analysis and reaction path are examined and discussed. Kinetic modeling of hydrogen combustion in stirred reactors demonstrates that with the currently adopted rate constants this mechanism is of major importance in rich hydrogen/air mixtures burning in stirred reactor between 1000 and 1400 K at pressures between 0.5 and 8 atm. The possibility of its existence and its relative importance are based on the correct evaluation of the rate constants of the key most sensitive reactions (3), (4), and

$$N_2H_2 + H = NNH + H_2 \qquad (6).$$

The choice of the rate constants of these reactions is discussed.

Available measurements of NO formation in hydrogen combustion in stirred reactors have been modeled and analyzed. They neither confirm nor contradict this novel route forming NO via N_2H_3, because these experiments have been conducted outside the range of conditions where this route is manifested.

NO Reburning in Fuel-Rich Low Pressure Propene Flames: Experiment and Modeling

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Three fuel-rich, non-sooting (Φ=1.5, 1.8, 2.3) laminar premixed propene flames doped with 1.0% and 0.1% NO at 50 mbar were investigated by laser induced fluorescence and analyzed with flame calculations to contribute to the understanding of the reburn chemistry by using a C_3 hydrocarbon fuel in extension of most previous studies, which were restricted to C_1- and C_2-hydrocarbons as fuels.

Temperature was measured by laser induced fluorescence of seeded NO. This technique was also applied to determine absolute NO concentrations. NO mole fractions in the exhaust were found to be reduced to 45, 20 and 10% of the initial doping level for Φ=1.5, 1.8, and 2.3, respectively. Flame calculations were performed using three different kinetic models for the NO_x chemistry, namely mechanisms of Konnov, of Miller and Melius, and the GRI 2.11 mechanism. All models predict the NO concentration profiles reasonably well for these stoichiometries. Differences between the model predictions are noted for the HCN and N_2 concentrations, especially for the flame with Φ=2.3. Reaction flow analysis with respect to NO reveals the importance of NO consumption by HCCO under these conditions, whereas consumption by CH_i radicals is of minor influence. However, differences in product distributions and reaction rates of some important reactions are found between the models, especially for reactions of CH_2+NO and for HCCO+NO. Differences are also observed in the formation and consumption channels of HCN leading to different product distributions.

Experimental Evaluation of Corona Discharge Reactor for Removal of Soot Particles and NO_x in Diesel Engine Exhaust

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We have experimentally evaluated the application of a corona discharge reactor apparatus to reduce the concentrations of diesel soot particles and NO_x in the exhaust gas of a conventional diesel engine. The exhaust gas is treated by passing through a corona discharge collector for diesel soot particles (CCDS) and a corona reactor for NO_x removal (CBNR) in a high voltage electric field. The CCDS is designed to collect soot particles electrically on a central electrode and accumulated soot is removed by a regeneration technique. In a corona reactor CRNR, the NO is oxidized to NO_2 and reacts with H_2O contained in the gas, NO_x decreases as a results of HNO_3 formation. In our study the effects of corona voltage, current, and inlet temperature on the exhaust gas on the soot removal rate and the NO_x removal rate are considered. In addition, a prototype reactor, which couples CCDS with CRNR for soot and NO_x removal, is proposed in this study. We found that (i) the soot removal rate of 70-90% is obtained at corona input power of 3 W (15 kV) to 8 W (23 kv). (ii) the central electrode of the CCDS can be regenerated by controlled burning process. (iii) NO_x removal rate of 95% was observed at an input power of 80 W.

MODELING OF SOOT IN TURBULENT DIFFUSION FLAMES OF METHANE

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The aim of this work is to test several soot models together with a detailed simulation of a turbulent diffusion flame. Predicting soot in turbulent flames is a highly challenging task. Nevertheless, it is an important task as we know that most industrial combustion processes are turbulent. A thorough understanding of the soot formation process as well as the ability to model this process is necessary to develop more efficient and cleaner combustion equipment.

This work presents results from numerical simulations of a turbulent diffusion flame of methane. The predictions are validated against experimental data provided by Brookes and Moss. The simulations include coupled models for turbulence, combustion, radiation, and soot. All simulations are performed with a general-purpose CFD code which has been developed at our department over the last two decades. The interaction of turbulence and chemical reactions is modeled by the Eddy Dissipation Concept (EDC) developed by Magnussen and co-workers. EDC is based on the assumption that the chemical reactions occur in the regions where the dissipation of turbulence energy takes place. The EDC combustion model is used in conjunction with the complete GRI-Mech 3.0 reaction mechanism. When modeling soot formation and oxidation, predicting the correct flame temperature is of crucial importance. To ensure a satisfactory representation of the flame temperature, a radiation model is implemented in the program.

Three different soot models are used in the simulations, the original EDC soot model proposed by Magnussen, a more detailed soot model developed by Lindstedt and co-workers, and a modified EDC soot model. Results from simulations with the three different soot models are discussed and compared with experimental data.

DATA FOR THE SOOT MODEL VALIDATION: LII AND SHIFTED VIBRATIONAL CARS MEASUREMENTS

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The reduction of pollutants in technical combustion systems is an important challenge for the design of new combustion systems. In the past the focus has been on gaseous species like NO_x. Now increasing efforts are aiming at the processes contributing to soot formation and oxidation. There are two main approaches towards a comprehensive understanding of these reactions: the experimental determination of physical properties in sooting flames and theoretical modeling of the underlying chemical processes. For the development of the soot model a validation by experimental data in simplified combustion systems is necessary. An extensive pool of validation data is desirable that contains different equivalence ratios, pressures and fuels. Besides the measurement of soot volume fractions, a precise temperature determination is important for the model validation since it has a strong influence on the gas phase precursor chemistry of soot formation.

For the validation of the soot model, well defined experimental boundary conditions of the flame under study are necessary. By a new burner design, we were able to separate soot growth and oxidation by preventing the entrainment of secondary air into the soot region of the flame. The investigated flame is surrounded by a coflame of equivalence ratio $\Phi=1$. Thus the inner sooting flame is shielded to the outside by a hot gas film.

First results are presented for a laminar premixed ethene/air flame at different equivalence ratios in the range of $2<\Phi<3$ for pressures up to 0.4 Mpa. Soot volume fractions are measured by 2-D Laser

Induced Incandescence (LII), excited by a lasersheet at 532 nm. Calibration of the LII signal is obtained by simultaneous dual beam extinction measurements with a HeNe laser.

N_2 vibrational CARS spectroscopy is an established technique for temperature measurements in flames. In conventional vibrational N_2 CARS, using the frequency-doubled output of the Nd:YAG at 532 nm as the pump and a dye laser as the broadband Stokes source, the method becomes very difficult as soon as the soot concentration within the flame rises. Under these conditions the C_2 Swan band at 473 nm interferes and disturbs the N_2 signal spectra. By modifying the conventional excitation scheme and using a narrowband dye laser instead of the 532 nm of the Nd:YAG laser, we were able to shift the CARS spectrum to lower wavenumbers out of this C_2 Swan band interference. First measurements demonstrate the improved access of sooting flames for temperature determination by shifted vibrational CARS spectroscopy (SV-CARS).

COMPUTATIONAL AND EXPERIMENTAL STUDIES OF SMALL AROMATIC RADICAL REACTIONS OF RELEVANCE TO INCIPIENT SOOT FORMATION

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Small aromatic radicals, such as phenyl and napthyl, have been shown by kinetic modeling of soot formation to be key reactive species responsible for the formation of polycyclic aromatic hydrocarbons, precursors to soot. In an attempt to establish a kinetic database for these small aryl radical reactions, in the past several years we have measured the rate constants for C_6H_5 reactions with a number of hydrocarbons and combustion species using different complementary spectroscopic techniques. We have also carried out quantum chemical calculations (by ab initio MO up to 8 heavy atoms and by hybrid DFT for larger systems) to elucidate their reaction mechanisms as well as to interpret the measured rate constants using TST or RRKM theory.

LASER INDUCED INCANDESCENCE MEASUREMENTS IN TURBULENT ETHYLENE DIFFUSION FLAMES

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Instantaneous, spatially-resolved measurements of soot within turbulent diffusion flames is necessary for model development and testing. In the paper presented here, experimental results are shown using laser induced incandescence for quantified soot volume fraction measurements within turbulent ethylene/air diffusion flames.

Two-dimensional LII images reveal a dramatic increase in soot volume fraction (f_v) with increasing O_2 ambient concentration. With increased f_v, the spatial extent of soot containing regions also increases, resulting in a decrease in the soot intermittency. This trend is borne out by plots of the spatially integrated soot intermittency. Radial profiles of f_v reveal both an increase and contraction of the soot containing region, consistent with the qualitative indications suggested by the LII images and C_2 emission images. PDFs of f_v quantify the fluctuation in this quantity and reflect the impact of shear layer mixing upon soot processes.

These findings are consistent with the time-averaged flame location and its associated effect upon the gas density and temperature into which the fuel-jet issues as determining the rate and extent of soot inception and growth. Analogous to laminar diffusion flames, the reaction zone resides outside of the fuel-rich region, beyond the shear layer., The results presented here illustrate that the proximity of the reaction front to the shear layer induced turbulent mixing dramatically affects the soot loading, its fluctuation and spatial distribution. Increasing the stoichiometric mixture fraction by increasing the O_2 ambient concentration causes laminarization of the potential core. Yet the locally higher concentrations of hot combustion products offsets the reduced shear layer mixing and accelerates soot inception and growth, yielding a higher f_v . Finally, the radial variation in f_v reflects the intermittency and randomness in the turbulent mixing as measured by soot inception and growth.

KINETICS OF SOOT NANOPARTICLE OXIDATION

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Soot emission from combustion sources is dictated by the competing surface processes of growth and oxidation. We have developed a new experimental method to conduct surface chemistry and extract surface kinetic rates from mobility-area selected soot particles generated in flames and internal combustion engines. These mono-area particles are characterized for changes in surface area during a controlled high temperature oxidation (or condensation) using on-line nanoparticle characterization instrumentation. Quantitative kinetic information for surface oxidation rates can then be determined by changes in surface area. This technique is being used to determine the rate of soot oxidation as a function of temperature, particle size, and fuel type. We believe these to be the first measurements of soot oxidation kinetics that have been conducted on mono-surface area particles. The results will be used to evaluate existing kinetic models.

NUMERICAL SIMULATION OF THERMO-IONIZATION OF SOOT PARTICLES AND ITS EFFECT ON SOOT GROWTH IN LAMINAR PREMIXED FLAMES

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The effect of thermo-ionization on soot particle growth is analyzed by detailed kinetic modeling of low-pressure premixed acetylene flames. The model considers fuel oxidation, formation and growth of polycyclic aromatic hydrocarbons, and soot particle inception, coagulation, and heterogeneous surface reactions.

In this work we investigate the production of charged particles by thermo-ionization as well as coagulation and surface reactions of these particles. Neutral particles and particles carrying one negative or positive charge are considered. The collision enhancement due to van der Waals, image and electrostatic forces between the particles is rigorously accounted for in the numerical model. The particle size distribution functions for both neutral and charged particles are calculated using the method of moments. The model is validated using measurements of number densities and relative soot volume fractions of charged and neutral particles in a low-pressure laminar premixed C_2H_2/O_2 flame.

The sensitivities on electron concentrations and heterogeneous surface reactions are studed in a laminar premixed $C_2H_2/O_2/Ar$ flame. The results show that the omission of particle thermo-ionization does not lead to significant errors in the simulation of soot formation in acetylene flames, as long as the nature of the surface reactions between charged particles and gaseous molecules remains to be the same as for neutral particles. This result can be generalized to most laboratory laminar premixed and counterflow diffusion flames with flame temperature not exceeding 2100 K. Only if the surface reaction between charged particles and gas molecules is enhanced should the thermo-ionization potentially play a role in particle mass growth. Regardless, the uncertainty associated with the omission of thermo-ionization is significantly smaller than the uncertainties in the kinetics of particle inception and surface growth.

Predissociation in the Hydrocarbon Flame Bands of HCO

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We use large-scale multiconfiguration self-consistent field/configuration interaction calculations to characterize the predissociation mechanism of the B^2A' state of HCO through conical intersection with the X^2A' ground state, the hydrocarbon flame band. We locate two regions of intersection: the first represents a highly bent HCO that is 8 kcal/mol energetically lower than the B-state minimum, with a barrier height of 26 kcal/mol. Energy points on the B^2A' potential surface connecting these extrema were also calculated. This region emphatically illustrates the feasibility of a nonradiative decay mechanism consistent with latest experimental findings of purely vibronic coupling mechanism. The second region of intersection represents a confluence of three linear ($^2\sigma^+$-$^2\pi$) states crossings, 53 kcal/mol below the B-state minimum. A barrier about 21 kcal/mol above the state equilibrium structure is located and assigned to the entrance channel of H-CO($^3\pi$).

Vinyl Radical: Visible Spectroscopy and Excited State Dynamics

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The vinyl radical, $C_2H_3(A^2A''\leftarrow X^2A')$ spectrum has been measured between 530 and 360 nm using cavity ringdown spectroscopy. Optimal rotational constants and linewidths were determined for the first three vibrational bands by modeling the spectrum as an asymmetric top. About 1200 cm^{-1} above the excited state origin the model can no longer match the experimental spectra and linewidths become very broad, signifying the appearance of new dynamics involving a non-planar isomer. Our best-fit results combined with previously published ab initio calculations offer new information on the radical's structure and unimolecular dynamics. The change in rotational constants and linewidths with increasing vibrational excitation provides further insight into vinyl's geometric deformation and unimolecular dissociation. Additional information on the dynamics in the excited and electronic state of the vinyl radical has been obtained by studying the same transition in the perdeuterated isomer of vinyl.

$NH_2(A^2A_1)$ Radiative Lifetimes

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The $NH_2(A^2A_1$-$^2B_1)$ absorption involves an electronic transition from a linear ground state to a bent excited state. This geometry change favors transitions to highly excited bending levels in the excited state. Radiative lifetimes were measured for bands excited between 750 and 410 nm reaching as A^2A_1 levels as low as $\nu_2=3$ and as high as $\nu_2=17$. The results resolve a long standing disagreement between experimental data in the literature. Radiative lifetimes range from 67 to 5 µs, decreasing with increasing vibrational excitation. The variation of lifetime with vibrational level generally agree with the predictions of Jungen, Hallin and Merer, however, there are significant deviations for the highest and lowest vibrational levels.

MECHANISM OF THE REACTION CH_4+O($^1D_2$)®CH_3+OH, STUDIED BY ULTRAFAST AND STATE-RESOLVED PHOTOLYSIS/PROBE SPECTROSCOPY OF THE CH_4ˣO_3 VAN DER WAALS COMPLEX

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The mechanism of the reaction $CH_4+O(^1D_2)\rightarrow CH_3+OH$ was investigated in state-resolved and time-resolved experiments. Ultraviolet pulses photolyzed ozone in the $CH_4{\cdot}O_3$ van der Waals complex to produce $O(^1D_2)$. The ensuing reaction with CH_4 was monitored by laser induced fluorescence through the OH(A←X) transition. In the state-resolved measurements, the distribution of OH(v=0,1;J) states, P_{obs}(v,J) was determined using a tunable, high resolution laser. In the time-resolved measurements, an ultrafast laser system was used to monitor the appearance of these OH states at probe wavelengths centered between 307 and 316 nm. Because the ultrafast probe laser was spectrally broad, many rovibrational states were probed simultaneously. At each probe wavelength, multiple appearance rates were evident in the fluorescence signal, and the ratio of these components varied with probe wavelength. These data are most consistently fit using a three-mechanism model. The OH appearance signals, at all probe laser wavelengths, were best fit with time constants of $\tau_{fast}\approx0.2$ ps, $\tau_{inter}\approx0.5$ ps and $\tau_{slow}\approx5.4$ ps. The slowest of these three is the rate predicted by statistical theory for dissociation of a vibrationally excited methanol intermediate (CH_3OH^*) after complete intramolecular energy redistribution following insertion of $O(^1D_2)$ into CH_4. Under the assumption that the mechanism producing OH at the statistical rate would be characterized by a statistical prior, P_{obs}(v,J), was decomposed into three components, each with a linear surprisal. Dissociation of a CH_4O^* intermediate before complete energy randomization was identified as producing OH at the intermediate rate and was associated with a population distribution with more rovibrational energy than the slow mechanism. The third mechanism produces OH promptly with a cold rovibrational distribution, indicative of a colinear abstraction mechanism. From the decomposition of P_{obs}(v,J), it was possible to predict the fraction of signal associated with each mechanism at each probe wavelength in the ultrafast experiment, and the predictions proved consistent with measured appearance signals.

CAVITY RINGDOWN SPECTROSCOPY APPLIED TO AN ATMOSPHERIC PREMIXED FLAT FLAME FOR ABSOLUTE SPECIES CONCENTRATIONS

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In order to gather insight into the reaction mechanisms of combustion processes, several laser diagnostic techniques can be applied to determine absolute molecular densities in atmospheric flames. However, many of these lack the required sensitivity of the quantitative data and are not sufficiently accurate. Therefore, we have used Cavity Ringdown Spectroscopy (CRDS) to study a laminar flame under different conditions at atmospheric pressure. In recent years the sensitivity of the method has also been demonstrated in the area of combustion research, mainly on low pressure flames. We have studied the presence and location of several different species in a CH_4/air flat flame at atmospheric pressure.

The concentration profiles of CH, OH, HCO and CH_2 in a burner stabilized flat flame of a premixed CH_4/air burner have been measured. Since at atmospheric pressure the CH radical is present only in a very narrow area at the flame front, specific problems due to the finite size of the laser beam and thermal deflection are encountered which make the investigation particularly challenging. The excitation laser beam was matched to the cavity modes with an ICCD camera to obtain a good spatial resolution.

The CH radicals are excited from the $X^2\Pi_{3/2}$ to the $A^2\Delta$ state at 430 nm. After corrections for the spatial intensity distribution and bandwidth of the laser beam CH density distributions are obtained for two

different stoichiometries in a burner stabilized flame. Signal-to-noise ratios indicated that total CH densities down to $8 \cdot 10^{10}$ cm^{-3}, corresponding to 3 ppb can be detected easily. The local flame temperature is derived from measured Boltzmann distributions. The results are compared to model calculations using GRI-Mech 2.11. The predicted CH peak concentrations are 28% higher and are shifted by 0.2 mm to a larger distance above the burner surface. Also, the computed CH maximum appears at a higher temperature, further away from the burner.

OH density distributions have been measured via the $X^2\Pi$ to the $A^2\Sigma^+$ transition at 307 nm. Comparisons with direct absorption and bi-directional LIF measurements and numerical simulations show a reasonable to good agreement both for concentrations and derived temperatures. In addition, data on the minority species CH_2 and HCO have been collected by absorption in the 620 nm wavelength range and compared to results from model calculations. It was found that the sensitivity was limited by the large temperature gradient resulting in a deflection of the laser beam.

CH and Formaldehyde Structures in Partially-Premixed Methane/Air Coflow Flames

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The structures of CH and CH_2O in partially premixed, atmospheric pressure, methane/air Bunsen-type coflow flames are examined with planar laser induced fluorescence (LIF) imaging. LIF excitation strategies are chosen to minimize the temperature dependent partition function variation for CH_2O and to maintain signal strength for CH while eliminating Rayleigh scattering background in the CH images. Spatially resolved excitation and fluorescence scans form detection strategies to isolate CH and CH_2O. The structures of the premixed inner cone of the Bunsen flame are determined from two-dimensional images of the LIF for fuel/air stoichiometries, $1.36 \leq \Phi \leq 3.0$. The formaldehyde structure appears inside the CH in the inner flame cone for the moderately fuel rich stoichiometries typical of well-tuned, blue flames used in natural gas appliances. At richer inner flame stoichiometries the CH structure begins to disappear and by $\Phi = 2.7$ no CH LIF can be distinguished from the background. However, the formaldehyde exhibits a distinct inner flame cone structure even for very fuel rich conditions, with a width increasing as the inner cone becomes richer. The variation in the relative concentrations of CH and formaldehyde are replicated in a one-dimensional model of the inner cone reaction zone with a flame velocity matching to the experiment. The prediction of the absolute CH concentration agrees within a factor of two with the measured value. LIF images of CH and CH_2O were observed for a variety of flame inserts, with accompanying exhaust probe measurements of CO and NO. Metal objects are often inserted into appliance flames to reduce NO_x emissions and improve heat transfer. We observe that a variety of metal inserts reduced NO, increased CO, and broadened CH_2O structures in the flames studied here.

A Microelectrochemical NO_x Sensor for Combustion Exhausts

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A chemiresistive micromachined NO_x sensor for combustion exhaust application has been developed. The sensor uses a thin (100 nm) amorphous tungsten oxide film the resistance of which is sensitive and selective to NO_x in the presence of other combustion products. Conventional CMOS fabrication techniques were used to build the sensor on a silicon wafer. The thin tungsten oxide film is deposited on a plate that is released from the silicon wafer using a wet bulk etching process that forms an inverted pyramidal cavity under the plate providing excellent thermal insulation. A polysilicon heating element and an aluminum temperature sensing plate are incorporated into the released plate to provide closed-loop temperature control of the plate and sensing film. The tungsten oxide film was deposited by sputtering of a pure WO_3 target in an oxygen-rich environment. Rutherford backscattering was used to measure film stoichiometry, which was found to be $WO_{3\pm0.08}$.

The completed NO_x sensor was characterized in a calibration facility consisting of gas flow control panel, a Pyrex test cell and a NO_x chemiluminescence analyzer. The flow panel accurately meters three gas streams so that the composition of the gas in the test cell can be varied. The sensor sensitivity and speed of response were determined by measuring film resistance as a function of NO mole fraction and film temperature. These measurements show that the response of the thin film to NO in $NO/N_2/O_2$ mixtures was independent of the O_2 mole fraction. The response of the sensor to NO can be modeled by a Freundlich isotherm that relates film resistance to the partial pressure of NO by

$$R_{film} = R_0 \text{constant} \ (1 + P_{NO}{}^m)$$

where R_0 is the film resistance in the absence of NO and m is a fitting constant that is a function of temperature. The sensitivity of the sensor decreases and the sensor time constant decreases as the film temperature increases. Phase transformation and grain growth in the tungsten oxide film limits the operating temperature to below 315 °C. The 90%-response time decreases from 4 minutes at room temperature to approximately 1.7 minutes at 80 °C, the highest film temperature tested. In the film temperature range investigated, the sensor accuracy is approximately ±5 ppm for 300 ppm NO, and the minimum detectivity is approximately 5 ppm.

In combustion products, the strongest interference to NO on chemiresistive sensors is due to CO, which has a similar valence outer shell as NO. To examine the selectivity of the sensor, the sensor was exposed alternately to NO, CO and combinations of these species. No detectable change in sensor resistance was found when it was exposed to 500 ppm CO, and the sensor response to NO did not change in the presence of CO.

The Structure of Kinetic Rate Equations Leads to Steady States, Radical Pools and Low Dimensional Manifolds

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The chemical kinetics mechanisms of combustion reactions frequently lead to steady states and radical pools. Steady states and radical pools are established quickly. Maas and Pope have taken advantage of this to devise numerical schemes where the progress of the reaction is calculated using only a few variables that change slowly. The remainder of the variables are effectively held at their steady state value. Frequently one or two variables are sufficient to reproduce the heat release with reasonable accuracy. (Lam and Goussis have developed a related method.)

This work links steady states and radical pools to the structure of the chemical kinetic rate equations. Although the rate equations are non-linear, and solutions of non-linear differential equations often exhibit interesting behavior, steady states and radical pools arise even from linearized equations such as those used to analyze the induction period of hydrogen or methane oxidation. Hirschfelder, and later Winslow, pointed out that chemical kinetic rate equations take the form

$$d[X_i]/dt = F - G[X_i] \qquad (1)$$

where F and G are sums of non-negative terms, each of which represents a forward or reverse reaction rate, one for each reaction involving species X_i. Note that all terms involving X_i are negative and that F does not contain terms in species X_i. The local solution of Eq. 1, assuming F and G are approximately constant is

$$[X_i] = F/G + ([X_i]_0 - F/G)\exp[-G(t-t_0)]$$

It is clear that every X_i, including reactants and products, has a steady state $[X_i]=F/G$ which is approached with a time constant 1/G.

If the dominant terms in F are proportional to intermediate concentrations $[X_k]_{k\neq i}$ then two or more species concentrations are coupled. For example, in the H_2+Br_2 reaction one gets

$$[H] = (k_1[H_2]/k_2[Br_2])[Br]$$

constituting a radical pool. In the case of branching chain reactions, substitution of steady states into terms in F yields terms proportional to X_i whose sum is greater than $G[X_i]$, leading to growth of the radical pool. Thus, steady states and radical pools arise out of the structure of Eq. 1.

The Low Dimensional Manifold method of Maas and Pope was applied to the H_2+O_2 reaction mechanism. The resulting numerical eigenvalues were close, but not identical, to the time constants obtained from Eq. 1 and by substituting steady states into the rate equation for [H].

LAMINAR NON-PREMIXED FLAME CALCULATIONS OF METHANE WITH HIGHLY PREHEATED AIR

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Flameless Oxidation (FLOX) is a combustion regime which incorporates recirculation of hot combustion products to the oxidant stream (vitiation) to oxidize the fuel without having a flame. The concept is being explored commercially by Japanese scientists in a full scale furnace. This regime achieves low emission of NO_x and CO pollutants and improved fuel savings. Its application can also be tailored to low calorific fuels, which are often produced in chemical processes or vented from coal mines. The combustion in these devices takes place at reduced temperature in the range of 1100-1700 K. It is characterized by a flat thermal field, minor temperature fluctuations and when optimized, there are no visible or audible flame, hence the name.

In this poster the laminar nonpremixed flame is investigated computationally using the OPPDIF code. Methane is used as fuel, while the air was diluted with combustion products (CO_2 and H_2O) to alter the oxygen levels in the oxidant stream. The chemical kinetics mechanism used in the calculations has been optimized for low temperature methane oxidation. It consists of 51 species and 200 reactions including nitrogen oxidation. It is worth mentioning that the GRI 2.1 mechanism do not sustain methane flames at temperatures lower than 1400 K. Current investigation using the GRI 3.0 mechanism is underway.

The methane nonpremixed laminar flame calculations under preheated oxidizer stream conditions and at low strain rate exhibit the following characteristics:

1. An increase in the oxidizer stream temperature broadens the reaction zone substantially and exhibits a distributed reaction regime;
2. At temperatures higher than 1200 K and low oxygen levels (<4% by volume) the combustion regime resembles that of the FLOX regime;
3. The OH radical at the FLOX conditions does not seem to be of importance while CH_2O species increases substantially under these conditions.

This work is a first in a series that aim at enhancing the understanding of FLOX combustion. In particular, issues such as Damkohler number effects on the structure and stability of the flame will be explored. A burner is being built to investigate laminar and turbulent nonpremixed flames under the FLOX regime. This burner will be used to conduct measurements or reactive scalars using single-point Raman-Rayleigh-LIF measurements at Sandia National Laboratory later in the year.

TEMPERATURE DEPENDENCE OF RADICAL RECOMBINATION BY PHOSPHORUS BASED FLAME SUPPRESSANTS

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The influence of dimethyl methyl phosphate, DMMP($O=P(OCH_3)_2CH_3$), on OH concentrations was studied in atmospheric pressure, nonpremixed flames of CH_4 versus $O_2/N_2/Ar$ in an opposed-jet burner. OH concentrations were measured using laser induced fluorescence (LIF). Phosphorus-based flame suppressants, such as DMMP, are believed to inhibit flames via catalytic radical recombination of H and OH. In this study the "inhibition effectiveness" of DMMP is evaluated in terms of reduction in OH concentration due to its presence. The influence of flame temperature on inhibition effectiveness is an important consideration in evaluating the feasibility of new chemically-active flame inhibitors and has direct bearing on synergistic effects observed when these inhibitors are combined with physical agents such as N_2, CO_2, or water. A series of four flames with differing adiabatic flame temperatures were studied. Flame temperature was varied by changing the proportions of N_2 and Ar in the oxidizer side diluent, while maintaining 21% (by vol) O_2 and thus a constant stoichiometric mixture fraction of 0.055. Adiabatic flame temperatures ranged from 2260 K (79% N_2 - 21% O_2, note: this is slightly hotter than a typical methane/air flame due to 100 °C reactant preheat necessary to keep DMMP in the gas phase) to 2558 K (79% Ar - 21% O_2). In the absence of DMMP, measured OH profile widths show good agreement with OPPDIF calculations made using GRI Mech 3.0 for all flames considered. Corrections to raw LIF data for Boltzmann factor and local quenching environment are performed using temperature and major species data from the calculations. Peak OH concentrations from calculations of the undoped flames are used to calibrate the corrected LIF measurements. Measurements of DMMP's inhibition effectiveness are not affected by this final calibration as they are expressed in terms of the fractional reduction in the total OH population relative to the undoped flame.

Addition of 572 ppm of DMMP to the oxidizer stream for the N_2-O_2 versus CH_4 flame results in a 23% reduction in total OH population (integrated across flame width). In the substantially hotter Ar-O_2 versus CH_4 flame the same loading results in a reduction of less than 3%. Earlier extinction measurements conducted with the same configuration in which both temperature and stoichiometric mixture fraction were varied, indicated the same trend of decreasing effectiveness (measured in terms of reduction in global extinction strain rate) with increasing temperature. This temperature dependence implies that a mixture of inert and phosphorus-based inhibitors would interact synergistically as the physical agent cools the flame, thus increasing the efficiency of the chemically-active component. In the current work, the inhibition effectiveness of DMMP is observed to vary linearly with adiabatic flame temperature over the range of conditions considered. A short extrapolation of the data indicates that at an adiabatic flame temperature near 2600 K the inhibition effectiveness of phosphorus-based agents will be reduced to zero, with flame promotion occurring at higher temperatures. These results are compared to calculations made using a proposed mechanism for DMMP decomposition and phosphorus radical chemistry. It should be noted that these strained laminar flames have calculated peak temperatures nearly 300 K cooler than the adiabatic flame temperatures, thus the flame promotion temperature threshold predicted by the experiments is actually in the vicinity of 2300 K.

KINETICS OF THE REACTION Al(^{2}P)+SF_6 IN THE TEMPERATURE RANGE 300-600 K

N.L. Garland and J.K. Parker, Chemistry Division, Naval Research Laboratory, 4555 Overlook Ave., Washington, DC 20375, Fax (202) 404-8119, e-mail: nancy.garland@nrl.navy.mil, chjkp@normandy.nrl.navy.mil (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

The kinetics of the gas phase reaction of ground state ^{2}P aluminum atoms with sulfur hexafluoride have been studied over the temperature range 300-600 K in a resistively heated flow reactor. Aluminum atoms are generated by photolysis of trimethylaluminum at 248 nm and are monitored by laser induced resonance-fluorescence at 394.4 nm. Most experiments were carried out at about 50 torr total pressure using argon as a buffer gas. Temperatures were obtained, in separate experiments, from rotational spectra of AlO using the ($B^2\Sigma^+$-$X^2\Sigma^+$),(1,0) band. The reaction rate constant is pressure-independent between 5-50 torr total pressure at room temperature, consistent with a simple atom abstraction mechanism. The data indicate a 2.4 kcal/mole activation energy for the reaction. The implications of these results on models of aluminum particle combustion in fluorine containing environments will be discussed.

THE REACTION, $CH+O_2$, AS A SOURCE OF $OH(A^2S^+)$ IN ATOMIC FLAMES AND ITS RATE COEFFICIENT BETWEEN 295 AND 800 K

S.A. Carl, M. Van Poppel and J. Peeters, Department of Chemistry, University of Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium (Presented as a Work-in-Progress Poster at the *28th International Symposium on Combustion,* Held in Edinburgh, Scotland, August 2000).

Minor pathways, producing electronically excited species such as CH*, OH*, C_2* and HCO*, in a small group of highly exothermic reactions are responsible for nearly all the visible and near ultraviolet emissions from hydrocarbon flames. The relatively short lifetime of these electronically excited products establishes the direct proportionality of chemiluminescence intensity to their rate of formation. Consequently, chemiluminescence emissions, in flames of suitable geometry, are able to provide highly spatially resolved information on, for example, specific chemical pathways and fuel consumption rates. Meaningful interpretation of flame chemiluminescence measurements however, requires knowledge at least of the reaction, or reactions, leading to formation of the electronically excited species. Further, if the rate coefficients for such reactions are known, absolute determination of the concentration product of the reactants is possible.

Although the reaction of CH with O_2 has long been the prime candidate as the source of OH chemiluminescence in many flames, it has not been definitely established.

In this work we have measured chemiluminescence emission, $OH(A^2\Delta\text{-}X^2\Pi)$ intensities from a low-pressure C_2H_2/O_2/O/H flame, set up in an isothermal fast-flow reactor, were correlated against CH and O_2 concentrations as a function of reaction time and under a variety of helium-diluted C_2H_2/O_2/O/H mixtures. The species concentrations were measured using molecular-beam sampling threshold-ionization mass spectroscopy. Under all conditions the OH chemiluminescence intensity was found to be directly proportional to the concentration product, $[CH][O_2]$ over a range of 2 decades. It is argued that the reaction $CH+O_2$ is the major, if not the only, source of electronically excited OH in such flames. We are also carrying out detailed, absolute calibrations for [CH] and $[OH(A^2\Delta)]$ that will allow accurate determination of the rate coefficient of the title reaction over the temperature range 295 to 900 K.

REACTION DYNAMICS OF CH_2, C_2H, C_2H_3 WITH O_2 AND NO STUDIED BY TIME-RESOLVED FTIR SPECTROSCOPY

F. Wong, H. Su, H. Wang, M. Huang and B. Chen, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China 100080 (Presented as a Work-in-Progress Poster at the *28th International Symposium on Combustion,* Held in Edinburgh, Scotland, August 2000).

Elementary reactions of CH_2, C_2H and C_2H_3 radicals with O_2 and NO have been studied by Time-Resolved FTIR Spectroscopy. The nascent reaction products are directly observed within ten collisions. For each reaction, several channels are identified. The intermediate and the transient state are also studied by ab initio or DFT calculations.

Electronically state-specific $CH_2(X^3B_1)$ and $CH_2(a^1A_1)$ radicals were produced by laser photolysis of ketene at 351 and 308 nm, respectively. Vibrationally excited products of CO(v<8), CO_2(v<7), H_2CO, H_2O formed in $CH_2(X^3B_1)+O_2$ reaction and CO formed in $CH_2(a^1A_1)+O_2$ reaction have been observed. For each reaction, three possible channels have been verified.

For CH_2+NO reaction, the primary products of vibrationally excited CO, HCO, HOCN, OH and NH_2 were detected for the first time and four reaction channels have thus been identified. Theoretically, a doublet potential energy surface is characterized. On the potential energy surfaces, both the $CH_2(X^3B_1)$+NO and $CH_2(a^1A_1)$+NO systems reach a crucial intermediate OCHNH via a CNO ring-closure and ring-open process.

Vibrationally excited products of CO, HCO, HNC and HCN were observed from the C_2H+NO reaction. Three exothermic reaction channels leading to HCN+CO, HNC+CO and CN+HCO are identified, verifying an association-elimination reaction mechanism. The nascent product of CO and CO_2 were observed for the reaction of C_2H with O_2. The experimental observation supports that the reaction is a rapid and fierce process, preferably forming CO and HCO.

Three channels of the $C_2H_3+O_2$ reaction, $HCO+H_2CO$, CH_3+CO_2 and $C_2H_2+HO_2$, have been verified. For the C_2H_3+NO reaction, the nascent products of H_2CO and HCN have been observed.

Kinetics of the Reactions of Hydrocarbon Radicals with CH_3. The Reactions $R+CH_3$ ($R=C_2H_5$, n-C_3H_7, n-C_4H_9, C_3H_5, C_3H_3)

V.D. Knyazev and I.R. Slagle, Department of Chemistry, The Catholic University of America, Washington, DC 20064 (Presented as a Work-in-Progress Poster at the *28th International Symposium on Combustion,* Held in Edinburgh, Scotland, August 2000).

Rate constants of the gas phase reactions of five saturated and unsaturated hydrocarbon radicals with CH_3

(1) $C_2H_5+CH_3 \rightarrow$ products, $k_1=5.86\times10^{-5}\ T^{-2.11}\exp(-394K/T)$, 301-800 K

(2) *n*-$C_3H_7+H_3 \rightarrow$ products, $k_2=1.15\times10^{-8}\ T^{-0.84}\exp(+45K/T)$, 297-600 K

(3) *n*-$C_4H_9+CH_3 \rightarrow$ products, $k_3=1.19\times10^{-6}\ T^{-1.55}\exp(-131K/T)$, 297-520 K

(4) C_3H_5(allyl)$+CH_3 \rightarrow$ products, $k_4=6.46\times10^{-8}\ T^{-1.08}\exp(-90K/T)$, 301-800 K

(5) C_3H_3(propargyl)$+CH_3 \rightarrow$ products, $k_5=2.91\times10^{-4}\ T^{-2.27}\exp(-561\ K/T)$, 301-800 K

were measured over wide ranges of temperatures (see above) at densities of He in the interval (3-36)$\times10^{16}$ atoms cm^{-3} by the Laser Photolysis/Photoionization Mass Spectrometry technique. Units of rate constants are cm^3 $molecule^{-1}$ s^{-1}.

The $R+CH_3$ rate constant measurements were performed under pseudo-first order conditions using a method similar to that used earlier by Niiranen and Gutman. CH_3 and R radicals were produced by the 193 nm photolysis of acetone

$$CH_3C(O)CH_3 \rightarrow 2\ CH_3+CO \qquad (6)$$

and the simultaneous photolysis of the corresponding precursor of the radicals. Under the experimental conditions used in the current work, reaction 6 accounts for more than 95% of acetone photolysis. Concentrations of radical precursors were selected to create a large excess of initial concentrations of methyl radicals over the total combined concentration of all the remaining radicals formed in the system, so that the $R+CH_3$ process under study dominates all other minor reactions of R. The temporal evolution of the ion signals of R, CH_3 and $CH_3C(O)CH_3$ was monitored in real time. Under each set of conditions, the values of the rate constants were obtained from the observed radical decay profiles. The temperature dependences obtained can be represented with modified Arrhenius expressions.

Complexity of Kinetics and Product Channels for $C_2H_3+O_2$

P.R. Westmoreland, Department of Chemical Engineering, University of Massachusetts, 159 Goessmann, Box 33110, 686 N. Pleasant, Amherst, MA 01003, Fax (530) 327-9669, e-mail: westm@ecs.umass.edu (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

Vinyl radical (C_2H_3) can react with O_2 by a large number of pathways. Because its other dominant reactions are decomposition or addition for molecular weight growth, quantitative rate constants are important for designing furnaces and turbines to form or prevent pollutant PAH and soot. Two direct H-transfer reactions give $C_2H_2+HO_2$ while combination leads to about twenty more channels because of chemical activation. Only a few prove to be important, as determined by a combination of ab initio quantum chemistry [largely BAC-MP4/6-31G(d,p)//UHF/6-31G(d)], quantum reaction theory [Bimolecular Quantum-RRK and RRKM] and experiments. Dominant product channels are predicted to be CH_2O+CHO, C_2H_3O+O, and $C_2H_2+HO_2$, but at high temperatures, the dominant channel is to revert to reactants, causing the rate constant toward products to decrease dramatically with increasing temperature.

Kinetics and Mechanism for the Reaction of Phenyl Radical with Formaldehyde

Y.M. Choi, W. Xia, J. Park and M.C. Lin, Department of Chemistry, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, Fax (404) 727-6586, e-mail: ymchoi@euch4e.chem.emory.edu (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

The kinetics and mechanism for the $C_6H_5+CH_2O$ reaction was investigated by the Cavity Ringdown Spectrometric and Pulsed Laser Photolysis/Mass Spectrometric methods at temperatures between 298 and 1083 K. The measured values of the rate constants obtained by the two different methods agree closely, suggesting that the $C_6H_5+CH_2O=C_6H_6+CHO$ reaction is the dominant channel. A weighted least-squares analysis of the two sets of data gave

$$k=8.55x10^4\ T^{2.19}exp[-19/T]\ cm^3\ mol^{-1}\ s^{-1}$$

for the temperature range studied. The mechanism for the $C_6H_5+CH_2O$ reaction was also elucidated with a quantum-chemical calculation employing a hybrid density functional theory using the aug-cc-PVTZ basis set. The rate constant calculated for the H-abstraction process using the predicted 0.8 kcal/mol barrier with a small tunneling correction agrees closely with the experimental result, particularly at low temperatures.

Mechanism and Absolute Rate Coefficients for the Reaction of Phenyl Radical with Acetylene: A Theoretical Study

I.V. Tokmakov and M.C. Lin, Department of Chemistry, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, Fax (404) 727-6586, e-mail: itokmak@emory.edu (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

The theoretical analysis of the PES for the $C_6H_5+C_2H_2$ addition reaction revealed that chemically activated adducts can undergo several isomerization pathways in competition with well-known deactivation and H-elimination channels. Thus formed isomeric C_8H_7 vinylic, aromatic and bicyclic radicals can serve as active agents in the mass growth reactions with C_2H_2 and other light unsaturated hydrocarbons and radicals. The latter processes are relevant to the PAH formation in hydrocarbon combustion at moderate temperatures. The calculated G2M energetics agree well with the available experimental data. Our predicted heat of the $C_6H_5+C_2H_2=C_6H_5CCH+H$ reaction, ΔH_{0K}= -10.9 kcal/mol, lies within the uncertainty limits of the experimental value of -12.2 kcal/mol and the calculated barrier for the addition step at 0 K, 3.8 kcal/mol, is in reasonable agreement with the experimental activation energy, 3.1 kcal/mol.

Kinetics of the Reactions of C_6H_5 with $C_6H_5C_2H_x$(x=1,3)

G.J. Nam, I.V. Tokmakov, J. Park and M.C. Lin, Department of Chemistry, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, Fax (404) 727-6586, e-mail: ginam@euch4e.chem.emory.edu (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

The reactions of C_6H_5 with phenylacetylene ($C_6H_5C_2H$) and styrene ($C_6H_5C_2H_3$) have been investigated using the cavity ringdown technique in the temperature range 297-410 K. The weighted least squares analysis for each reaction gave rise to the following rate constant expressions in units of cm^3/(mol s):

$$k(x=1) = 1.0x10^{13}exp(-1224/T) \text{ and}$$
$$k(x=3) = 2.0x10^{13}exp(-1294/T).$$

The theoretical study of these reactions at the B3LYP/cc-pvdz level of theory showed that the phenyl radical addition at the beta position is the most favorable reaction mode. The products of C_6H_5 beta-addition to $C_6H_5C_2H_x$ feature benzyl-type free radicals stabilized by an overlap with aromatic pi-orbitals (for both x=1 and x=3). The calculated barriers at 0 K for the addition step are 1.5 and 0.7 kcal/mol for $C_6H_5C_2H$ and $C_6H_5C_2H_3$, respectively.

Rate Constants for H + O_2 + M ® HO_2 + M at Room Temperature in Seven Bath Gases and at High Temperature in N_2, Ar and O_2

J.V. Michael, M.-C. Su, J.W. Sutherland and J.J. Carroll, Chemistry Division, Argonne National Laboratory, Argonne, IL 60439 (Presented as a Work-in-Progress Poster at the *28th International Symposium on Combustion,* Held in Edinburgh, Scotland, August 2000).

The third-order reaction H + O_2 + M was directly studied in seven bath gases. The detection method for H-atom depletion was H-atom atomic resonance absorption spectrometry. In these experiments, the measured room temperature rate constants for H_2O, N_2, O_2, Ar, Kr, Ne and He are 50(±5), 4.32(±0.28), 3.13(±0.06), 2.16(±0.14), 2.10(±0.10), 1.40(±0.04), and 1.80(±0.07), all with 2σ errors and in units of 10^{-32} cm^6 $molecule^{-2}$ s^{-1}, respectively. These room temperature values were then combined with T-dependent values (450-700 K) obtained in N_2, Ar, and O_2 using the Laser Photolysis-Shock Tube technique. For these three cases, the T-dependence can be adequately described by

N_2, $k(T) = 4.82(\pm1.03) \times 10^{-29}\ T^{-1.23(\pm0.04)}$

Ar, $k(T) = 1.26(\pm0.27) \times 10^{-29}\ T^{-1.12(\pm0.04)}$

and O_2, $k(T) = 1.57(\pm0.38) \times 10^{-29}\ T^{-1.09(\pm0.04)}$

in cm^6 $molecule^{-2}$ s^{-1} units.

These values are in substantial agreement with Mueller, Yetter and Dryer and also with Bates, Hanson, Bowman and Golden. Unimolecular rate theory is used to rationalize the present and previous results.

Ab Initio Molecular Orbital and Rate Constant Calculations for the NCO + NO Reaction

R. Zhu and M.C. Lin, Department of Chemistry, Emory University, 1515 Pierce Dr., Atlanta, GA 30322, Fax (404) 727-6586, e-mail: rszhu@euch4e.chem.emory.edu (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

The mechanism for the NCO + NO reaction has been studied using the modified G2 method (G2M) in conjunction with RRKM calculations. The results indicate that the reaction occurs primarily via singlet potential surface according to the following steps: (1) NCO + NO↔OCNNO→2 N_2O + CO; (2) NCO + NO↔OCNNO→2 *cyc*-NNC(O)O→2 N_2 + CO_2. Both processes take place via very tight transition states. The decomposition of the intermediate OCNNO to products N_2O + CO is energetically less favorable (by about 8.2 kcal/mol) than the cyclization process of forming *cyc*-NNC(O)O intermediate. The calculated reaction heat for step (1) and (2) are 64.3 and 150.2 kcal/mol, respectively, which are in agreement with experimental values of 65 and 153 kcal/mol. The total rate constant and product branching ratio have been calculated employing canonical variational RRKM theories.

Rotational and Translational Energy Transfer in Collisions Between Highly Vibrationally Excited Pyrazine and CO

Q. Ju, N. Seiser, E. Sevy, J.-Y. Cai and G. Flynn, Department of Chemistry, Columbia University, New York, NY 10027, Fax (212) 860-6988 (Presented at the *220th National Meeting of the American Chemical Society*, Held in Washington DC, August 2000).

High resolution infrared transient absorption spectroscopy is used to study translational and rotational energy transfer in collisions between highly vibrationally excited pyrazine (E = 41000 cm^{-1}) and the bath gas CO. Vibrationally hot pyrazine was excited via 248 nm excimer laser pumping followed by rapid non-radiant decay to its ground electronic state. The nascent CO(v = 0,J = 21 ~ 36) populations and their recoil velocities were measured following single collisions with energized pyrazine. High level-density field to state energy transfer probabilities and rates were determined over the temperature range 243 to 364 K. The energy transfer distribution function, P(E,E′), and the collision mechanism have been explored. Comparisons among Pyrazine/CO, Pyrazine/CO_2, Methylpyrazine/CO_2, and Perfluorobenzene/CO_2 provide important insights into the energy transfer mechanism for molecules with chemically significant amounts of energy.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

SEPTEMBER 3-7, 2000

16th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY
Prague, Czech Republic.

Information: S. Urban, UFCH JH Academy of Sciences of the Czech Republic, Dolejskova 3, Prague, Czech Republic, CZ-18223, (420) 2-6605-3635, Fax (420) 2-858-2307, e-mail: praha2k@jh-inst.cas.cz, http://www.chem.uni-wuppertal.de/conference/

SEPTEMBER 3-8, 2000

11th EUROPEAN CONFERENCE ON DIAMOND, DIAMOND-LIKE MATERIALS, CARBON NANOTUBES, NITRIDES AND SILICON CARBIDE
Porto, Portugal.

Information: L. Reed, Conference Secretariat, e-mail: e.reed@elsevier.co.uk, http://www.elsevier.nl/locate/diamondconf

SEPTEMBER 4-8, 2000

EUROPEAN AEROSOL CONFERENCE
Trinity College, Dublin, Ireland.

Information: The Aerosol Society, P.O. Box 34, Portishead, Bristol, BS20 7FE, UK, http://www.aerosol-soc.org.uk

SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

SEPTEMBER 10-15, 2000

1st INTERNATIONAL SYMPOSIUM ON MICROGRAVITY RESEARCH AND APPLICATION IN PHYSICAL SCIENCES AND BIOTECHNOLOGY
Sorrento, Italy.

Information: ESTEC, Conference Bureau, P.O. Box 299, 2200 AG Noordwijk, The Netherlands, (71) 5655005, Fax (71) 5655658, e-mail: confburo@estec.esa.nl

SEPTEMBER 10-15, 2000

7th DURHAM CONFERENCE ON PLASMA SOURCE MASS SPECTROMETRY
Durham UK.

Information: G. Holland, Department of Geological Sciences, Science Laboratories, South Road, Durham City DH1 3LE, UK, e-mail: tannersd@sciex.com, (44) 191-374-2526, Fax (44) 191-374-2510.

SEPTEMBER 12-14, 2000

3rd UNITED KINGDOM MEETING ON COAL RESEARCH AND ITS APPLICATIONS
Birmingham, UK.

Information: H.J. Graham, Power Technology Centre, Radcliffe-on-Soar, Nottingham NG11 0EE, UK, 44(0)115-936-2460, Fax 44(0)115-936-2205, e-mail: helen.graham@powertech.co.uk

SEPTEMBER 13-16, 2000

2nd INTERNATIONAL CONFERENCE ON INORGANIC MATERIALS
Santa Barbara CA.

Information: Sarah Wilkinson, Conference Secretariat, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford, UK OX5 1GB, 44(0) 1865 843691, Fax 44(0) 1865 843658, e-mail: sm.wilkinson@elsevier.co.uk, http://www.elsevier.com/locate/im2000

SEPTEMBER 18-20, 2000

13th INTERNATIONAL SYMPOSIUM ON GAS FLOW AND CHEMICAL LASERS AND HIGH POWER LASER CONFERENCE
Florence, Italy.

Information: C. Pescucci, Fax 39(0) 55-233-7755, e-mail: gcl-hpl@ino.it, www.ino.it/GCL-HPL or www.es.titech.ac.jp/~kkasuya/gcl-web/index.html

SEPTEMBER 19-21, 2000

THE HYDROGEN ENERGY FORUM 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

SEPTEMBER 23-26, 2000

ASME Fall Technical Conference of the Internal Combustion Engine Division
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

SEPTEMBER 24-26, 2000

1st Romanian International Conference on Analytical Chemistry
Brasov, Romania.

Information: G.L. Radu, University of Bucharest, Faculty of Chemistry, 4-12, Elisabeta Blvd., Bucharest, Romania 703461, 40(1) 220 77 80/220 79 09, Fax 40(1) 220 76 95, e-mail: lucian@ibd.dbio.ro

SEPTEMBER 29-30, 2000

Four Corners Section Fall Meeting of the American Physical Society
Fort Collins CO.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 2-5, 2000

ICALEO 2000, International Conference on Applied Laser Applications and Electrooptics
Dearborn MI.

Information: E. Cohen, Laser Institute of America, (800) 345-2737 or (407) 380-1553, Fax (407) 380-5588, http://www.laserinstitute.org

OCTOBER 2-6, 2000

5th International Aerosol Symposium
Budapest, Hungary.

Information: N.N. Belov, Hungary, 1046 Budapest, Deak F. u., 26/a Belov N., Tel/Fax (36) 1-3791251, e-mail: belov@inext.hu, http://www.ias.inext.hu/uk-ias5-spo.htm.

OCTOBER 4-5, 2000

FLAMMABLE AND COMBUSTIBLE LIQUIDS SYMPOSIUM
Baltimore MD.

Information: SFPE, 7314 Wisconsin Ave Suite, Bethesda, MD 20814, (301) 718-2910, Fax (301) 718-2242, http://www.sfpe.org/educational_programs.html

OCTOBER 8-11, 2000

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 13-14, 2000

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Toledo, OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

OCTOBER 17-20, 2000

BEIJING INTERNATIONAL CONFERENCE ON APPLIED COMPUTATIONAL FLUID DYNAMICS
Beijing, China.

Information: Z. Tianyuan, Institute of Applied Physics and Computational Mathematics, (86) 10-62374357, Fax (86) 10-62010108, e-mail: zty@mail.iapcm.ac.cn, http://www.ciccst.org.cn/acfd

OCTOBER 19-20, 2000

SAMPLING, ON-SITE ANALYSIS AND SAMPLE PREPARATION CONFERENCE
Pittsburgh PA.

Information: B. Sherman, PACS, 409 Meade Dr., Coraopolis, PA 15108, (724) 457-6576 or (800) 367-2587, Fax (724) 457-1214, e-mail: hnpacs@aol.com, http://members.aol.com/hnpacs/pacs.htm

OCTOBER 19-21, 2000

CONFERENCE ON PHOTOPHYSICS AND PHOTOCHEMISTRY
Oeiras, Portugal.

Information: A. Macanita, ITQB, AP 127, Oeiras, Portugal, 2781-901, (351) 21-4411277, e-mail: pp2000@itqb.unl.pt, http://www.itqb.unl.pt/pp2000/

OCTOBER 20-21, 2000

NEW YORK SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Buffalo NY.

Information: M. DeMarco, Department of Physics, SUNY-Buffalo State College, 1300 Elmwood Ave., Buffalo, NY 14222, (716) 878-5230, e-mail: DemarcMJ@buffalostate.edu

OCTOBER 20-28, 2000

ANNUAL MEETING OF THE OPTICAL SOCIETY OF AMERICA AND THE INTERDISCIPLINARY LASER SCIENCE CONFERENCE
Providence RI.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf
Deadline: Abstracts Due by May 16, 2000

OCTOBER 22-27, 2000

198th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Phoenix AZ.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

OCTOBER 24-27, 2000

53rd ANNUAL GASEOUS ELECTRONICS CONFERENCE OF THE AMERICAN PHYSICAL SOCIETY
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 25-28, 2000

35th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
St Louis MO.

Information: C.D. Spilling, Department of Chemistry, University of Missouri, St. Louis, 80001 Natural Bridge Road, St. Louis, MO 63121 (314) 516-5313, Fax (314) 553-5342, e-mail: cspill@umsl.edu

OCTOBER 25-28, 2000

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Information: N.D. Byington, Customs Service Laboratory, 630 Sansome Street, Room 1429, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: byington@crl.com; or S. Rodriguez, Chemistry Department, University of the Pacific, Stockton, CA 95211, (209) 946-2598, Fax (209) 946-2607, e-mail: srodriguez@uop.edu

OCTOBER 28-29, 2000

JOINT FALL MEETING OF THE TEXAS SECTIONS OF THE APS, APPT AND ZONE 13 OF THE SPS
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 29-NOVEMBER 3, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Atlantic City NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710 (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

NOVEMBER 1-2, 2000

COMPUTATIONAL AND EXPERIMENTAL METHODS IN RECIPROCATING ENGINES
London UK.

Information: U. Otuonye, Conference and Events Department C587, Institution of Mechanical Engineers, 1 Birdcage Walk, London SW 1H 9JJ, UK, (0) 207-304-6864, Fax (0) 207-222-9881, e-mail: u_otuonye@imeche.org.uk

NOVEMBER 2-4, 2000

SOUTHEAST SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Starkville MS.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 3-4, 2000

9th CONFERENCE ON CURRENT TRENDS IN COMPUTATIONAL CHEMISTRY
Vicksburg MS.

Information: S.R. Allen, Jackson State University, Jackson, MS 39217, (601) 979-3723, e-mail: srallen@stallion.jsums.edu, http://www.ccl.net/cca/info/conferencelist/mess0665.shtml

NOVEMBER 3-5, 2000

8th CONFERENCE ON MOLECULAR NANOTECHNOLOGY
Bethesda MD.

Information: Foresight Institute, Box 61058, Palo Alto, CA 94306, (650) 917-1122, Fax (650) 917-1123, http://www.foresight.org/conference

NOVEMBER 3-8, 2000

PHOTONICS EAST
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:
- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 5-10, 2000

INTERNATIONAL SYMPOSIUM ON MULTIPHASE FLOW AND TRANSPORT PHENOMENA
Antalya, Turkey.

Topics will Include:
- Modeling of Multiphase Systems
- Transport Phenomena in Multiphase Systems
- Separation Phenomena, Processes and Equipment
- Measurement and Instrumentation
- Characteristic and Effective Properties of Multiphase Systems
- Bio-Aerosols and Bio-Systems
- Surface and Interfacial Phenomena
- Pollution Control Technology
- Clean Room Technology
- Multiphase Systems Applications
- Scaling Laws for Two-Phase Flow Phenomena
- Scaling Laws for Multiphase Flow

Information: D.M. Maron, Center for Technological Education Holon, POB 305, Holon 58102, Israel, (972) 3-502 6501, Fax (972) 3-502 6510, e-mail: barad_r@barley.cteh.ac.il, http://ichmt.me.metu.edu.tr/upcoming-meetings/MFTP-00/announce.html

NOVEMBER 5-10, 2000

UNITED ENGINEERING FOUNDATION CONFERENCE ON LEAN COMBUSTION TECHNOLOGY AND CONTROL
Santa Fe NM.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com http://www.engfnd.org/engfnd/conf.html, or from D. Dunn-Rankin, University of California at Irvine, CA, or R.K. Cheng, Lawrence Berkeley National Laboratory.

NOVEMBER 12-17, 2000

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Los Angeles, CA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

NOVEMBER 19-21, 2000

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 19-23, 2000

4th EUROMECH FLUID MECHANICS CONFERENCE
Eindhoven, The Netherlands.

Information: M.C.J. Tielemans, Fluid Dynamics Laboratory, Department of Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands, e-mail: info@efmc2000.tue.nl, http://www.efmc2000.tue.nl

NOVEMBER 27-DECEMBER 1, 2000

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

♦ NOVEMBER 28 - DECEMBER 1, 2000

2000 CHINA INTERNATIONAL ENVIRONMENT, RENEWABLES AND ENERGY EFFICIENCY EXHIBITION AND CONFERENCE
Beijing, China.

Information: CERE'2000 Secretariat, 1 Sandaojie, Jianguomenwai, Beijing 100022, PR China, (86) 10-6515-7760/5027, Fax (86) 10-6515-8442, e-mail: cisc@midwest.com.cn, web: www.ciscexpo.orgcn.net

DECEMBER 3-9, 2000

6th RIO SYMPOSIUM ON ATOMIC SPECTROMETRY
Concepcion and Pucon, Chile.

Information: C.G. Bruhn, Departamento de Analisis Instrumental, Facultad de Farmacia, Universidad de Concepcion, P.O. Box 237, Concepcion, Chile, (56) 41-204252, Fax (56) 41-231903, e-mail: cbruhn@udec.cl, http://www.udec.cl/6riosymp/

♦ DECEMBER 4-6, 2000

21st CENTURY EMISSIONS TECHNOLOGY
London UK.

Information: S. Love, Conferences and Events Department C588, Institution of Mechanical Engineers, 1 Birdcage Walk, London SW1H 9JJ, 44(0) 20-7973-1312, Fax 44(0) 20-7222-9881, e-mail: s_love@imeche.org.uk, web: www.imeche.org.uk

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

JANUARY 8-11, 2001

39th AIAA Aerospace Sciences Meeting and Exhibit
Reno NV.

Information: S.X. Ying, MC 078-0421, The Boeing Company, 2401 E. Wardlow Rd., Long Beach, CA 90807, (562) 982-2113, Fax (562) 496-6647, e-mail: susan.x.ying@boeing.com, http://www.aiaa.org

JANUARY 14-19, 2001

Gordon Research Conference on Molecular Energy Transfer
Harbortown Resort, Ventura CA.

Information: J. Bowman, Department of Chemistry, Emory University, 1515 Pierce Drive, Atlanta, GA 30322, e-mail: bowman@euch3g.chem.emory.edu, http://www.grc.uri.edu

♦ JANUARY 14-19, 2001

15th Winter Fluorine Conference
St. Petersburg Beach FL.

Information: G.B. Hammond, Department of Chemistry, University of Massachusetts, Dartmouth, MA 02747, (508) 999-8865, Fax (508) 910-6918, e-mail: ghammond@umassd.edu; W.B. Farnham, DuPont Central R&D, Experimental Station, P.O. Box 80328, 328/205, Wilmington, DE 19880, (302) 695-2459, Fax (302) 695-9799, e-mail: william.b.farnham@usa.dupont.com

♦ JANUARY 19-22, 2001

13th Sanibel Conference on Mass Spectrometry: Informatics and Mass Spectrometry
Sanibel Island FL.

Information: American Society for Mass Spectrometry, 1201 Don Diego Avenue, Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org

♦ JANUARY 20-26, 2001

Photonics West: Optoelectronics 2001, LASE 2001, BIOS 2001 and Electronics Imaging 2001
San Jose CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

FEBRUARY 4-8, 2001

European Winter Conference on Plasma Spectrochemistry
Lillehammer, Norway.

Information: Y. Thomassen, NIOH, P.O. Box 8149 DEP, Oslo, Norway, N-0033, (47) 23-19 53 20, Fax (47) 23-19 52 06.

♦ FEBRUARY 15-20, 2001

AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE ANNUAL MEETING AND SCIENCE INNOVATION EXHIBITION
San Francisco CA.

Information: AAAS Meetings Office, 1200 New York Ave., N.W., Washington, DC 20005, (202) 326-6450, Fax (202) 289-4021, e-mail: aaasmeeting@aaas.org, website: http://www.aaas.org/meetings

FEBRUARY 18-23, 2001

GORDON RESEARCH CONFERENCE ON CHEMICAL REACTIONS AT SURFACES
Harbortown Resort, Ventura CA.

Information: J.C. Hemminger, Department of Chemistry, University of California, Irvine, CA 92697, e-mail: jchemmin@uci.edu, http://www.grc.uri.edu

FEBRUARY 25 - MARCH 2, 2001

GORDON RESEARCH CONFERENCE ON GASEOUS IONS
Ventura Beach Hotel, Ventura CA.

Information: P. Armentrout, Chemistry Department, 315 S. 1400 E. Rm 2020, University of Utah, Salt Lake City, UT 84112, (801) 581-7885, Fax (801) 581-8433, e-mail: armentrout@chemistry.utah.edu, http://www.grc.uri.edu/programs/2001/gaseous htm

MARCH 4-8, 2001

THE PITTSBURGH CONFERENCE, PITTCON 2001
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 5-8, 2001

SOCIETY OF AUTOMOTIVE ENGINEERS WORLD CONGRESS
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-1830, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MARCH 11-16, 2001

GORDON RESEARCH CONFERENCE ON MODERN DEVELOPMENTS IN THERMODYNAMICS
Ventura CA.

Information: R.S. Berry, Department of Chemistry, University of Chicago, 5735 South Ellis Avenue, Chicago, IL 60637, e-mail: berry@rainbow.uchicago.edu, http://www.grc.uri.edu

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 25-30, 2001

199th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Washington DC.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

♦ MARCH 25-28, 2001

2nd JOINT MEETING OF THE US SECTIONS OF THE COMBUSTION INSTITUTE
Oakland CA.

Topics will Include:

- Engine and Industrial Combustion
- Combustion Emissions
- Droplet and Spray Combustion
- Combustion Diagnostics
- Modeling and Numerical Simulation
- Chemical Kinetics

Information and Abstracts to W.J. Pitz, WSS/CI Secretary, L-370, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 423-0909, e-mail: pitz@llnl.gov
Deadline: 200 Word Abstract to be Submitted Preferably by e-mail by December 15, 2000. 5-Page Papers Due by March 23, 2001.

MARCH 25-30, 2001

CONFERENCE ON STATIONARY SOURCE SAMPLING AND ANALYSIS FOR AIR POLLUTANTS XXV
Destin FL.

Information: B.K. Hickernell, United Engineering Foundation, Three Park Ave., 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com, http://www.engfnd/engfnd/1aw.html

♦ APRIL 1-5, 2001

221st NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Diego CA.

Division of Fuel Chemistry:

- Reaction Mechanisms in Fuel Processing
  P.F Britt, Chemistry Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, (423) 574-5029, Fax (423) 576-5235, e-mail: brittpf@ornl.gov
- Coal Bed Methane
  P.C. Thakur, Consol Inc., R&D, 1027 Little Indian Creek Road, Morgantown, WV 26501, (304) 983-3207, Fax (304) 983-3209, e-mail: promodthakur@consolcoal.com
- Nitrogen Chemistry in Coal Utilization
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext 142, Fax (860) 528-0648, e-mail: marek@afrinc.com
- Carbon Products for Environmental Applications
  A. Lizzio, Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61801, (217) 244-4985, Fax (217) 333-8566, e-mail: lizzio@geoserv.isgs.uiuc.edu
- Fuels of the Future: Heavy Oil & Hydrogen for Fuel Cells
  R. Khan, Texaco Upstream Technology, 3901 Briar Park, Houston, TX 77042, (713) 954-6238, Fax (713) 954-6113, e-mail: khanmr@texaco.com
- Environmental Challenges for Fossil Fuel Combustion
  M.M. Maroto-Valer, Pennsylvania State University, Energy Institute, 405 Academic Activities Building, University Park, PA 16802, (814) 863-8265, Fax (814) 863-8892, e-mail: mmm23@psu.edu
- Solid Fuel Chemistry
  S.V. Pisupati, Department of Energy & Geo-Environmental Engineering, Pennsylvania State University, 124 Hosler Building, University Park, PA 16802, (814) 865-0874, Fax (814) 865-3248, e-mail: sxp17@psu.edu

Division of Physical Chemistry:

- Accurate Description of Low-lying Molecular States & Potential Energy Surfaces
  K.G. Dyall, Thermosciences Institute, NASA Ames Research Center, Mail Stop 230-3, Moffett Field, CA 94035, (650) 604-6361, Fax (650) 604-0350, e-mail: dyall@pegasus.arc.nasa.gov; M.R. Hoffmann, Department of Chemistry, University of North Dakota, (701) 777-2742, e-mail: Mark.Hoffmann@mail.chem.und.nodak.edu
- Methods for Addressing Time- & Length-Scale Problems in Molecular Simulations
  M. Challacombe, Theoretical Division, Los Alamos National Laboratory, Group T-12, Mail Stop B268, Los Alamos, NM 87545, (505) 665-5905, Fax (505) 665-3909, e-mail: MChalla@T12.LANL.Gov
- Molecular Photoelectron Spectroscopy
  P.M. Weber, Chemistry Department, Brown University, 324 Brook St., Providence, RI 02912, (401) 863-3767, Fax (401) 863-2594, e-mail: peter_weber@brown.edu; S.T. Pratt, CHM-Chemistry Division, Argonne National Laboratory, 9700 S. Cass Ave., Argonne, IL 60439, e-mail: stpratt@anl.gov
- Strong Field Chemistry: Molecules & Clusters in Intense Laser Fields
  R. Levis, Department of Chemistry, Wayne State University, Detroit, MI 48202, (313) 577-2597, e-mail: levis@chem.wayne.edu; A.W. Castleman Jr., Departments of Chemistry and Physics, Pennsylvania State University, (814) 863-3583, Fax (814) 863-5235, e-mail: awc@psu.edu

APRIL 16-20, 2001

SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

APRIL 16-20, 2001

XIII CARIBBEAN CONFERENCE ON CHEMISTRY AND CHEMICAL ENGINEERING
Havana, Cuba.

Information: A.J. Nunez Selles, Sociedad Cubana de Quimica, Ave 21&200, Atabey, Apdo. 16042, Havana, Cuba, CP 11600, (537) 218-178, Fax (537) 336-471, cqf@infomed.sld.cu

APRIL 23-27, 2001

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 28 - MAY 1, 2001

2001 APRIL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 29-MAY 2, 2001

INTERNAL COMBUSTION ENGINE DIVISION SPRING TECHNICAL CONFERENCE OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Philadelphia PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

MAY 7-9, 2001

CEC/SAE SPRING FUELS AND LUBRICANTS MEETING AND EXPOSITION
Orlando FL.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MAY 13-16, 2001

16th INTERNATIONAL CONFERENCE ON FLUIDIZED BED COMBUSTION
Reno NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 20-25, 2001

2nd INTERNATIONAL SYMPOSIUM ON ADVANCES IN COMPUTATIONAL HEAT TRANSFER
Cairns, Australia.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

MAY 20-25, 2001

10th INTERNATIONAL CONFERENCE ON FLUIDIZATION: FLUIDIZATION FOR SUSTAINABLE DEVELOPMENT
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

♦ MAY 27-31, 2001

49th ASMS CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS
Chicago IL.

Information: American Society for Mass Spectrometry, 1201 Don Diego Avenue, Santa Fe, NM 87505, (505) 989-4517, Fax (505) 989-1073, e-mail: asms@asms.org

MAY 27-JUNE 1, 2001

4th International Conference on Multiphase Flow
New Orleans LA.

Information: E.E. Michaelides, School of Engineering, Tulane University, New Orleans, LA 70118, e-mail: icmf@mailhost.tcs.tulane.edu, http://mail.eng.lsu.edu/icmf.2001/
Deadline: Abstracts Due by July 1, 2000

♦ MAY 29 - JUNE 1, 2001

ASME Fluids Engineering Summer Meeting: Symposium on Separated and Complex Flows III
New Orleans LA.

Information: B.E. Thompson, Department of Mechanics and Aerodynamics, Jonssen Engineering Center 2049, Rensselaer Polytechnic Institute, Troy, NY 12180, (518) 276-6989, Fax (518) 276-6025, e-mail: thompson@rpi.edu

MAY 30-JUNE 1, 2001

35th Middle Atlantic Regional Meeting of the American Chemical Society
Baltimore MD.

Information: L.J. Boucher, Towson University, Department of Chemistry, 8000 York Road, Towson, MD 21252-0001, (410) 830-3057, Fax (410) 830-4265, e-mail: lboucher@towson.edu

♦ JUNE 3-6, 2001

Symposium on Turbulent Mixing and Combustion
Kingston, Ontario, Canada.

Topics Will Include:
- Turbulent Mixing
- Mixing Dominated by Combustion
- Simulation and Modeling of Turbulent Mixing and Combustion
- Control of Mixing and Combustion
- Applications

Information: A. Pollard, Department of Mechanical Engineering, Queen's University at Kingston, ON, Canada K7L 3N6, (613) 533-2569, Fax (613) 533-6489, e-mail: pollard@me.queensu.ca, http://me.queensu.ca/~iutam
Deadline: Abstracts Due by February 1, 2001.

JUNE 4-7, 2001

46th ASME International Gas Turbine and Aeroengine Technical Congress, Exposition and Users Symposium
New Orleans LA.

Information: A. Layne, National Energy Technology Center, DOE, 3610 Collins Ferry Road, MS CO2, Morgantown, WV 26505, (304) 285-4603, Fax (304) 285-4469, e-mail: abbie.layne@netl.doe.gov, http://www.asme.org

JUNE 10-12, 2001

35th ASME NATIONAL HEAT TRANSFER CONFERENCE
Anaheim CA.

Information: C.B. Panchal, Energy Concept Co., Annapolis, MD 21401, (410) 266-6521, Fax (410) 266-6539, e-mail: cpanchal@aol.com, http://www.asme.org

JUNE 10-15, 2001

3rd INTERNATIONAL SYMPOSIUM ON RADIATIVE TRANSFER
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Anakara, Turkey, (90) 312-210-5214, Fax (90) 312-210-1331, http://ichmt.me.metu.edu.tr
Deadline: 4 Copies of Manuscript Due by December 15, 2000.

JUNE 11-13, 2001

JOINT CENTRAL/GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis Pharmaceuticals, 188 Howard Ave., Holland, MI 49424, (616) 392-2375 ext. 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 11-14, 2001

19th AIAA APPLIED AERODYNAMICS CONFERENCE
15th AIAA COMPUTATIONAL FLUID DYNAMICS CONFERENCE
31st AIAA FLUID DYNAMICS CONFERENCE
32nd AIAA PLASMADYNAMICS AND LASERS CONFERENCE
35th AIAA THERMOPHYSICS CONFERENCE
Anaheim CA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JUNE 13-15, 2001

JOINT 33rd CENTRAL/33rd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis, 188 Howard Avenue, Holland, MI 49423, (616) 392-2375 ext 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-16, 2001

56th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Seattle WA.

Information: S. Jackels, Department of Chemistry, Seattle University, 900 Broadway, Seattle, WA 98122, (206) 296-5946, Fax (206) 296-5786, e-mail: sjackels@seattleu.edu

JUNE 17-22, 2001

GORDON RESEARCH CONFERENCE ON ATMOSPHERIC CHEMISTRY
Salve Regina University, Newport RI.

Information: S.P. Sander, Jet Propulsion Laboratory, Mail Stop 183-901, 4800 Oak Grove Drive, Pasadena, CA 91109, e-mail: stanley.sander@jpl.nasa.gov, http://www.grc.uri.edu

JUNE 23-28, 2001

GORDON RESEARCH CONFERENCE ON ANALYTICAL CHEMISTRY
Connecticut College, New London CT.

Information: P.W. Bohn, Department of Chemistry, University of Illinois, 600 South Mathews, Urbana, IL 61801, e-mail: bohn@aries.scs.uiuc.edu, http://www.grc.uri.edu

JUNE 24-27, 2001

30th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Durham NH.

Information: H. Mayne, Chemistry Department, University of New Hampshire, (603) 862-1550, e-mail: howard.mayne@unh.edu

♦ JUNE 24-27, 2001

3rd ASIA-PACIFIC CONFERENCE ON COMBUSTION
Seoul, Korea.

Information: In-S. Jeung, School of Mechanical and Aerospace Engineering, Seoul National University, San 56-1, Shinrim-Dong, Kwanak-Ku, Seoul, 151-742, Korea, 82-2-880-7387, Fax 82-2-887-2662, e-mail: enjis@plaza.snu.ac.kr, http://aspacc.snu.ac.kr

JUNE 24-28, 2001

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JULY 1-6, 2001

GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS IN COMBUSTION
Mount Holyoke College, South Hadley MA.

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jay.jeffries@sri.com

JULY 8-11, 2001

37th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE
Salt Lake City UT.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JULY 8-13, 2001

GORDON RESEARCH CONFERENCE ON GRAVITATIONAL EFFECTS IN PHYSICO-CHEMICAL SYSTEMS
Colby-Sawyer College, New London NH.

Information: P.H. Steen, Department of Chemical Engineering, Cornell University, 346 Olin Hall, Ithaca, NY 14853, e-mail: phs7@cornell.edu, http://www.grc.uri.edu

JULY 8-13, 2001

GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT
Williams College, Williamstown MA.

Information: M. Johnson, Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520, e-mail: Mark.johnson@yale.edu, http://www.grc.uri.edu

JULY 9-11, 2001

COMBUSTION CHEMISTRY: ELEMENTARY REACTIONS TO MACROSCOPIC PROCESSES: FARADAY DISCUSSION NUMBER 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

♦ JULY 18-24, 2001

22nd INTERNATIONAL CONFERENCE ON PHOTONIC, ELECTRONIC AND ATOMIC COLLISIONS
Santa Fe NM.

Information: S. Datz, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, (865) 574-4984, Fax (865) 574-1118, e-mail: icpeac@phy.ornl.gov, http://icpeac2001.phy.ornl.gov.html

JULY 22-27, 2001

GORDON RESEARCH CONFERENCE ON HIGH TEMPERATURE CORROSION
Colby-Sawyer College, New London NH.

Information: P.Y. Hou, Lawrence Berkeley National Laboratory, Materials Science Division, 1 Cyclotron Road, MS 62-203, Berkeley, CA 94720, e-mail: pyhou@lbl.gov, http://www.grc.uri.edu

JULY 29-AUGUST 2, 2001

36th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Savannah GA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7057, Fax (212) 705-7143, http://www.asme.org

♦ JULY 29-AUGUST 3, 2001

18th INTERNATIONAL COLLOQUIUM ON THE DYNAMICS OF EXPLOSIONS AND REACTIVE SYSTEMS
Seattle WA.

Information: ICDERS Secretariat, Engineering Professional Programs, University of Washington, 10303 Meridian Ave North #301, Seattle, WA 98133.
Deadline: Submit Abstracts of Papers and Posters by February 1, 2001 to J.R. Bowen, University of Washington, 10303 Meridian Ave N #301, Seattle, WA 98133, (206) 616-8128, Fax (206) 543-2352, e-mail: icders@engr.washington.edu

AUGUST 6-10, 2001

INTERNATIONAL CONGRESS ON ANALYTICAL SCIENCES 2001
Yokohama, Japan.

Information: T. Sawada, Chairman, Department of Applied Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan 113-8656, (81) 3-5841-7236, ext. 7237, Fax (81) 3-5841-6037, e-mail: icas2001@laser.t.u-tokyo.ac.jp, http://wwwsoc.nacsis.ac.jp/jsac/icas2001/

AUGUST 19-24, 2001

1st INTERNATIONAL CONFERENCE ON ADVANCED VIBRATIONAL SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, 358-2-215-4295, Fax 358-2-215-4706, e-mail: icavs@abo.fi, http://www.abo.fi/icavs

AUGUST 19-24, 2001

GORDON RESEARCH CONFERENCE ON PHOTOACOUSTIC AND PHOTOTHERMAL PHENOMENA
Queen's College, Oxford UK.

Information: D. Fournier, UPMC/CNRS, Laboratoire d'Instrumentation, 10 Rue Vaugelin, Paris 75005, France, e-mail: fournier@optique.espci.fr, http://www.grc.uri.edu

AUGUST 20-24, 2001

13th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, (358) 2-265-4295, Fax (358) 2-265-4706, e-mail: icofts@abo.fi, http://www.abo.fi/icofts

AUGUST 26-30, 2001

222nd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Chicago IL.

Division of Fuel Science:

- Cofiring or Coprocessing Coal & Biomass
  J.T. Cobb, Jr., University of Pittsburgh, Chemical Engineering Department, 1137 Benedum Hall, Pittsburgh, PA 15261, (412) 624-7443, Fax (412) 624-9639, e-mail: cobb@engrng.pitt.edu
- Computer Modeling in Fuel Chemistry
  J. Mathews, Pennsylvania State University, Energy & Geo-Environmental Engineering Department, 151 Hosler Building, University Park, PA 16802, (814) 863-6213, Fax (814) 865-3248, e-mail: jpm10@psu.edu; M.T. Klein, Rutgers, State University of New Jersey, School of Engineering, Office of the Dean, B204, 98 Bret Road, Piscataway, NJ 08854-8058, (732) 445-4453, Fax (732) 445-7067, e-mail: mtklein@jove.rutgers.edu
- Fine Particulate (PM2.5) Formation & Emissons from Fuel Combustion
  C.M. White, Department of Energy, Federal Energy Technology Center, Mail Stop 94-212, P.O. Box 10940, Pittsburgh, PA 15236, (412) 386-5808, Fax (412) 386-4158, e-mail: cwhite@fetc.doe.gov
- Catalysis in Fuel Processing for Fuel Cell Application
  S.P. Katikaneni, Fuel Cell Energy, Advanced Technology Group, 3 Great Pasture Road, Danbury, CT 06813, (203) 825-6067, Fax (203) 825-6150, e-mail: skatikaneni@fce.com; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com; C. Song, Pennsylvania State University, Energy & Geo-Environmental Engineering, 206 Hosler Building University Park, PA 16802, (814) 863-4466, Fax (814) 865-3248, e-mail: csong@psu.edu
- Value-Added Carbon Products from Fossil Fuels
  F. Rusinko, Pennsylvania State University, Energy Institute 407 Academic Activities Building, University Park, PA 16802, (814) 863-8085, Fax (814) 865-8892, e-mail: fjr4@psu.edu; J.W. Zondlo, College of Engineering & Mineral Resources, Department of Chemical Engineering, P.O. Box 6102, Morgantown, WV 26506; B. Tomer, Department of Energy, Federal Energy Technology Center, 3610 Collins Ferry Road, P.O. Box 88, Morgantown, WV 26507.

- Mercury Emissions from Coal
  K. Katrinak, Microbeam Technologies, 1521-24th Avenue S., Suite B-2, Grand Forks, ND 58201, (701) 772-4482, Fax (701) 772-4099, e-mail: katrinak@badlands.nodak.edu; K. Galbreath, University of North Dakota, Energy & Environmental Research Center, P.O. Box 9018, Grand Forks, ND 58202, (701) 777-5127, Fax (701) 777-5181, e-mail: kgalbreath@eerc.und.nodak.edu
- General Fuel Chemistry
  S.V. Pisupati, Pennsylvania State University, Energy & Geo-Environmental Engineering, 124 Hosler Building, University Park, PA 16802, (814) 865-0874, Fax (814) 865-3248, e-mail: sxp17@psu.edu

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: Electronic Abstract Submissions (preferred) or 4 Hard Copies of 150-word Abstract (original on ACS Abstract Form) Due to Symposium Organizers by April 15, 2001. Preprints Due to Symposium Chairs by May 15, 2001.

SEPTEMBER 2-7, 2001

200th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY AND THE 52nd MEETING OF THE INTERNATIONAL SOCIETY OF ELECTROCHEMISTRY
San Francisco CA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

SEPTEMBER 23-27, 2001

52nd SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Savannah GA.

Information: G. Novotnak, Kemira Pigments, 104 Carlton Road, Savannah, GA 31410, (912) 652-1290, Fax (912) 897-1163, e-mail: george.novotnak@kemira.com

SEPTEMBER 23-27, 2001

6th WORLD CONGRESS OF CHEMICAL ENGINEERING: A NEW CENTURY OF CHEMICAL ENGINEERING
Melbourne, Australia.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325 or (800) 242-4363, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

SEPTEMBER 24-26, 2001

INTERNAL COMBUSTION ENGINE DIVISION FALL TECHNICAL MEETING OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Argonne IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

SEPTEMBER 24-27, 2001

INTERNATIONAL SAE FALL FUELS AND LUBRICANTS MEETING AND EXPOSITION
San Antonio TX.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

SEPTEMBER 24-28, 2001

5th WORLD CONFERENCE ON EXPERIMENTAL HEAT TRANSFER, FLUID MECHANICS AND THERMODYNAMICS
Thessaloniki, Greece.

Information: G.P. Celata, Conference Chairman, ENEA Casaccia, Via Anguillarese 301, I-00060 S.M. Galeria, Rome, Italy, (39) 06-30483905, Fax (39) 06-30483026, e-mail: celata@casaccia.enea.it, http://www.ing.unipi.it/exhft5
Deadline: Abstract Due by July 28, 2000

♦ SEPTEMBER 30-OCTOBER 5, 2001

11th INTERNATIONAL CONFERENCE ON COAL SCIENCE: EXPLORING THE HORIZONS OF COAL
San Francisco CA.

Information: D.A. Clarke, Power Technology, Radcliffe-on-Soar, Nottingham NG11 0EE, England, (0) 115-936-2452, Fax (0) 115-936-2363, e-mail: dave.clarke@powertech.co.uk

OCTOBER 5-12, 2001

28th ANNUAL MEETING OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 10-13, 2001

36th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

OCTOBER 14-18, 2001

6th International Symposium on Self Propagating High Temperature Synthesis
Haifa, Israel.

Information: I. Gotman, Technion-Israel Institute of Technology, Department of Materials Engineering, Technion, Haifa, Israel 32000, (972) 4-829-2112, Fax (972) 4-832-1978, e-mail: gotman@techunix.technion.ac.il, http://www.technion.ac.il/technion/materials/conferences.html

OCTOBER 14-19, 2001

International Symposium on Visualization and Imaging in Transport
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 16-19, 2001

57th Southwest Regional Meeting of the American Chemical Society
San Antonio TX.

Information: S.T. Weintraub, Department of Biochemistry, University of Texas Health Science Center, 7703 Floyd Curl Drive, San Antonio, TX 78284, (210) 567-4043, Fax (210) 567-5524, e-mail: weintraub@uthscsa.edu

OCTOBER 23-26, 2001

36th Western Regional Meeting of the American Chemical Society
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

♦ OCTOBER 28-31, 2001

37th Western Regional Meeting of the American Chemical Society
Santa Barbara CA.

Information: R.W. Hurst, Hurst & Associates, 9 Faculty Court, Thousand Oaks, CA 91360, fax/phone (805) 492-7764, e-mail: alasrwh@aol.com

NOVEMBER 26-30, 2001

Fall Meeting of the Materials Research Society
Boston MA.

Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

NOVEMBER 28-30, 2001

2001 SAE SMALL ENGINE TECHNOLOGY CONFERENCE AND EXPOSITION
Pisa, Italy.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org
Submit your abstract of up to 500 words by November 2, 2000 to Karin Bolcshazy, SAE International, 400 Commonwealth Drive, Warrendale, PA 15096, (724) 772-7179, Fax (724) 776-1830, e-mail: karinb@sae.org
The abstract should include a tentative paper title, authors and co-authors (full names, position, company address, email, telephone and fax numbers).

♦ DECEMBER 3-6, 2001

5th ASIA-OCEANIA SYMPOSIUM ON FIRE SCIENCE AND TECHNOLOGY
Callaghan, NSW, Australia.

Information: B.Z. Dlugogorski, Department of Chemical Engineering, The University of Newcastle, Callaghan, NSW 2308 Australia, 61-2-4921-6176, Fax 61-2-4921-6920, e-mail: cgbzd@alinga.newcastle.edu.au
Deadline: Submission of Full Papers by March 1, 2001.

♦ DECEMBER 9-14, 2001

14th AUSTRALASIAN FLUID MECHANICS CONFERENCE
Adelaide, Australia.

Information: 14th Australasian Fluid Mechanics Conference, Department of Mechanical Engineering, The University of Adelaide, SA 5005, Australia, (61) 8-8303 5397, Fax (61) 8-8303 4367, e-mail: afmc@mecheng.adelaide.edu.au, http://www.mecheng, adelaide.edu.au/14afmc/14afmc.htm

♦ JANUARY 6-11, 2002

2nd MEDITERRANEAN COMBUSTION SYMPOSIUM
Sharm El-Shaikh, Egypt.

Information: M.S. Mansour, Department of Mechanical Engineering, The American University in Cairo, Cairo, Egypt, Fax (202) 795-7565, e-mail: mansourm@aucegypt.edu

MARCH 18-22, 2002

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Indianapolis IN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 18-22, 2002

PITTCON 2000: THE PITTSBURGH CONFERENCE
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pitcon.org/

APRIL 7-12, 2002

223rd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Orlando FL.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ APRIL 29-MAY 1, 2002

5th INTERNATIONAL WORKSHOP ON CATALYTIC COMBUSTION
Seoul, Korea.

Topics will Include:

- Kinetics and Transport Processes in Catalytic Combustion
- Development of High Temperature Materials for Catalytic Combustion
- Application of Catalytic Combustion in Industrial Commercial and Residential Burners
- Commercialization of Low Emission Gas Turbine Catalytic Combustor

Information: Sung June Cho, Secretary, 5 IWCC, Korea Institute of Energy Research, 71-2, Jang-dong, Yusung-gu, Taejon 305-343, Korea, (82) 42-860-3613, Fax (82) 42-860-3133, e-mail: sjcho@kier.re.kr
Deadline: Submit Extended Abstract by July 31, 2001.

♦ MAY 5-8, 2002

7th CIRCULATING FLUIDIZED BED CONFERENCE
Niagara Falls, Canada.

Information: AICUL Consulting, e-mail: aicul-con@home.com

♦ JUNE 20-22, 2002

57th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY

Information: D. Cleary, Chemistry Department, Gonzaga University, Spokane, WA 99258, (509) 323-6631, e-mail: cleary@gonzaga.edu

♦ AUGUST 18-22, 2002

224th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Boston MA.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ OCTOBER 23-26, 2002

38th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Information: N.D. Byington, U.S. Customs Service Laboratory, 630 Sansome St., Room 1407, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: neal@byington.org

♦ NOVEMBER 13-17, 2002

53rd SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Charleston SC.

Information: G.P. Meier, Department of Pharmaceutical Sciences, Medical University of South Carolina, 280 Calhoun St., P.O. Box 250140, Charleston, SC 29425, (843) 792-8445, Fax (843) 792-0759, e-mail: meiergp@musc.edu

CURRENT BIBLIOGRAPHY RELEVANT TO
FUNDAMENTAL COMBUSTION
April 2000

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

85028.	Bain, R.L., R.P. Overend and K.R. Craig, "Biomass-Fired Power Generation," *Fuel Processing Technol.* 54, 1-16 (1998).	Biomass Fuels Energy Resource Potential
85029.	Baxter, L.L., T.R. Miles, T.R. Miles Jr., B.M. Jenkins, T. Milne, D. Dayton, R.W. Bryers and L.L. Oden, "The Behavior of Inorganic Material in Biomass-Fired Power Boilers: Field and Laboratory Experiences," *Fuel Processing Technol.* 54, 47-78 (1998).	Biomass Combustion Mineral Content Power Boiler Testing Experience
85030.	Porteous, A., "Energy from Waste: A Wholly Acceptable Waste Management Solution," *Appl. Energy* 58, 177-208 (1998).	Waste Combustion Energy Source Considerations
85031.	Daskalopoulos, E., O. Badr and S.D. Probert, "Economic and Environmental Evaluations of Waste Treatment and Disposal Technologies for Municipal Solid Waste," *Appl. Energy* 58, 209-255 (1997).	Waste Management Assessments
85032.	Bharadwaj, S.S., and L.D. Schmidt, "Catalytic Partial Oxidation of Natural Gas to Syngas," *Fuel Processing Technol.* 42, 109-127 (1995).	Syngas Formation CO,H_2 Catalytic Partial Oxidation Natural Gas/Steam
85033.	Edwards, J.H., and A.M. Maitra, "The Chemistry of Methane Reforming with Carbon Dioxide and Its current and Potential Applications," *Fuel Processing Technol.* 42, 269-289 (1995).	Synfuel Formation CO,H_2 CH_4/CO_2 Reforming Catalysts Carbon Product Overview

2. LIQUEFACTION/GASIFICATION

85034.	Holmen, A., O. Olsvik and O.A. Rokstad, "Pyrolysis of Natural Gas: Chemistry and Process Concepts," *Fuel Processing Technol.* 42, 249-267 (1995).	Liquefaction/ Gasification Natural Gas Pyrolysis Product Yields

85035.	Foulds, G.A., and B.F. Gray, "Homogeneous Gas Phase Partial Oxidation of Methane to Methanol and Formaldehyde," *Fuel Processing Technol.* 42, 129-150 (1995).	Partial Oxidation CH_4 Liquefaction CH_3OH,HCHO Formation
85036.	Tabata, K., Y. Teng, Y. Yamaguchi, H. Sakurai and E. Suzuki, "Experimental Verification of Theoretically Calculated Transition Barriers of the Reactions in a Gaseous Selective Oxidation of $CH_4/O_2/NO_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2648-2654 (2000).	Partial Oxidation $CH_4/O_2/NO_2$ Reaction Dynamics Energy Barriers Modeling
85037.	Choudhary, V.R., A.M. Rajput, B. Prabhakar and A.S. Mamman, "Partial Oxidation of Methane to CO and H_2 over Nickel and/or Cobalt Containing ZrO_2, ThO_2, UO_2, TiO_2 and SiO_2 Catalysts," *Fuel* 77, 1803-1807 (1998).	Partial Oxidation CH_4/O_2/Catalyst CO,H_2 Products Efficiencies
85038.	Deutschmann, O., and L.D. Schmidt, "Two-Dimensional Modeling of Partial Oxidation of Methane on Rhodium in a Short Contact Time Reactor," *Symp. (Int.) Combust. Proc.* 27, 2283-2291 (1998).	Synfuels Partial Oxidation CH_4/O_2/Rh 2-D Modeling
85039.	Hall, T.J., J.S.J. Hargreaves, G.J. Hutchings, R.W. Joyner and S.H. Taylor, "Catalytic Synthesis of Methanol and Formaldehyde by Partial Oxidation of Methane," *Fuel Processing Technol.* 42, 151-178 (1995).	Partial Oxidation CH_4 Liquefaction Catalytic CH_3OH,HCHO Formation
85040.	Chaouki, J., A. Gonzalez, C. Guy and D. Klvana, "Two-Phase Model for a Catalytic Turbulent Fluidized Bed Reactor: Application to Ethylene Synthesis," *Chem. Eng. Sci.* 54, 2039-2045 (1999).	Partial Oxidation Natural Gas/O_2 Catalytic C_2H_4 Synthesis FB Reactor 2-Phase Model
85041.	Hijikata, K., K. Ogawa and N. Miyakawa, "Methanol Conversion from Methane and Water Vapor by Electric Discharge (Effect of Electric Discharge Process on Methane Conversion)," *Heat Transfer - Asian Research* 28, 404-417 (1999).	Liquefaction CH_4/H_2O Vapor Discharge Method CH_3OH Yield
85042.	Stiller, A.H., D.B. Dadyburjor, J.-P. Wann, D. Tian and J.W. Zondlo, "Coprocessing of Agricultural and Biomass Waste with Coal," *Fuel Processing Technol.* 49, 167-175 (1996).	Liquefaction Coal/Biomass Wastes Mixture Effects
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Black Liquor
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(85191) Thermal Explosions, Preheated Combustible Gas, Injected Cool Spray Effects — Droplet Spray

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Radiation Heat
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Product PLIF AlO
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Joint PDFs
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Combustion
Magnetic Field
Generation
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Mechanism

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Decomposition
Pyrolysis/
Mass Analysis
Product Yields
Rate Constant

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Species Profiles
Flame Structure

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Products
Channels

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Continuous
Combustion

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PAH,PCB Formation
Metal Chloride
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Homo-/Heterogeneous
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CH_4/Air
Perovskites
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CH_4/O_2/Pd
Reaction Rates

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CO/O_2/Pt
Surface Modeling

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Catalytic
Partial Oxidation

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Catalytic
Reforming

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1-,2-Line Methods
Reliability

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Na,LIF
Laser Pumping
Complications
Assessments

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CH_4/Air Flame
Lower State
Rotational
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CH_4/Air
Rotational/
Laser Intensity
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CARS,H_2
2-Wavelength
Rotational
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n-$C_{16}H_{34}$/Air
(*t*-$C_4H_9)_2O_2$
Retarding
Promoting
Roles

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Kinetic Modeling
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Particle
Induced
CH_4/Air
Al_2O_3 Particles

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Mg(s)/CO_2
Ignition

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Ignition
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$N_2H_3(CH_3)/O_2$/Ar
Kinetic Modeling

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Combustion
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Modeling

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CH_4/Air/Pt
PLIF,OH
Measurements
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Ignition
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H_2/O_2/Pt
N_2 Diluted
Temperatures

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Instabilities
Measurements

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Confined
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Numerical
Algorithm

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Stability
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$CH_4(\nu)$
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Distributions
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Hypersonic
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Fluctuation
Covariances
New Modeling

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Nozzle Burner
PLIF
Surface Density

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Detonation
Initiation
Boundary
$H_2/O_2/Ar$
Supersonic Sphere

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Detonation
Wave Propagation
Orifice Plate
H_2/Air
Geometry
Length Scales

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Detonation
Propagation
Nonuniform
Mixtures
H_2/Air
Gradient Effects

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H_2/Air
Explosions

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3-D Structure
Flowfield
H_2/O_2

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Explosions
Flame
Instabilities
Cellular Structure
PLIF,OH
Schlieren
Measurements

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(See also Section 12 for Turbulent Flowfields)

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Combustion Flows
Surface Vibration
LDV
Flame Flicker
Measurements

(85307) Aircraft Emissions, Plume Modeling

Mixing/Entrainment

(85192) C_2H_2, C_2H_4, H_2/Air Initiation

Detonation
Flowfields

(85197)	H_2/O_2 3-D Structure, Hypersonic Flow	Detonation Wave Flowfield
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(85124)	RDX Ignition and Extinguishment, 2-D Profiles	PIV
(85102)	Velocities, Propagation, Measurements	Fe Particle Cloud Flame
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15. IONIZATION

(See also Section 26 for Ion Spectroscopy, Section 27 for Excited State Ionization, Section 40 for Dynamics of Ion-Molecule Reactions, Section 42 for REMPI, Section 44 for Ionic Structures and Section 46 for Thermochemical Values)

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(85646)	$CF_3COF + h\nu$, Product Quantum Yields	*c*-C_6H_{12},O_2 Additive Effects
(85324)	FBC Emissions Control, NO, SO_2 Levels	Ca Sorbents
(85300)	FBC, Domestic Wastes, Dioxin Control Effects	$CaCO_3$ Additive
(85327)	SO_2 Flue Gases Control, Sorbent Efficiencies	$Ca(OH)_2$/Fly Ash
(85331)	CCl_4/Ar, CCl_4/H_2/Ar Shock Tube Pyrolysis, Soot Formation, Growth Rates	$Fe(CO)_5$ Effects
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(85575)	DIAL Atmospheric Measurements	H_2O Vapor O_3 ,Aerosols
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FBC
Domestic Wastes
Emissions
$CaCO_3$ Addition
Effects

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Incineration
C_6Cl_6/O_2
Kinetic Parameters

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Pyrolytic
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C_6Cl_6/N_2
Product Analysis
Mechanisms

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Mineral Content
Distribution

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Emissions
HC,CO,CO_2
NO,SO_2
Bubbling FBC
I_2 Addition Effects

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Coal FBC
Air Excess Effects

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Fire Emissions
CO,CO_2,HCN,HCl
UHC,NO_x,SO_2
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Formation
Rich Flames
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Plume Modeling

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Wake Aerosol
Dynamics

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Aircraft Emissions
NO_x Formation
CH_4/Air
Modeling

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NO_x Formation
Pulverized Coal
Rank Effects
Measurements

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Coal Fired
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Numerical Model

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NO Formation/
Control
Coal Fueled
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Detailed Modeling
Controlling Parameters

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Unburned Carbon
Coal Type
Effects
Full Scale Testing

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Natural Gas/Air
Compositional
Effects
T,CO,O_2
Kinetic Modeling
Burning Velocities

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Turbulent
C_3H_8/Air
Diffusion
Kinetic Modeling

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Coal Quality
Effects

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NO Control
Natural Gas
LPG Reburn
Comparisons
Stirred Reactor
Mechanisms

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Reburn Method
Gas-on-Coal
Model
Validation

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NO_x Control
Natural Gas
Reburn Method
Mixing Model
Effects

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C_3H_6 Interaction
Stirred Reactor
Measurements
Kinetic Modeling

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NO_x Control
Reburn Method
Wood Potential
Measurements

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NO_x ,SO_x
Flue Gas
Scrubbing
Designs
Review

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NO_x ,SO_2 Control
Corona Discharge
Method
Efficiencies

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Emissions Control
FBC
Ca Sorbents
SO_2 ,NO
Levels

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N_2O Control
CFBC
C_3H_8 Afterburning
Emissions Effects

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SO_2 Control
FBC
Capture Performance
Modeling
Reliability

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SO_2 Control
Flue Gases
$Ca(OH)_2$ /Fly Ash
Sorbents
Efficiencies

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Carbon Microcoils
Formation
Ni Catalyzed
C_3H_8 Pyrolysis
Method

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Spherical Carbon
Onion Structured
Pyrolytic Graphite/
Shock Tube
Formation

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Soot,PAH
Particulate
Formation
Combustion
Pyrolysis
Kinetic Modeling

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Soot Formation
CCl_4 /Ar
CCl_4 /$Fe(CO)_5$ /Ar
CCl_4 /H_2 /Ar
Shock Tube
Pyrolysis
Growth Rates

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Soot Growth
CH_4 /O_2
H Atom
Measurements

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Soot Formation
CH_4 /O_2
O_2 Enriched Air
C_2H_2 ,PAH
Addition Effects

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Diamond Formation
C_2H_2/O_2 Flame
Growth Rates
$(CH_3)_2CO$ Effects

85344. Wolden, C.A., R.F. Davis, Z. Sitar and J.T. Prater, "Low Temperature Deposition of Optically Transparent Diamond Using a Low Pressure Flat Flame," *Diamond Related Mater.* 6, 1862-1867 (1997).

Diamond Formation
C_2H_2/O_2 Flame
Glass Substrates
Quality

85345. Kumar, S., and M. Malhotra, "Growth of Polycrystalline Diamond Films on Stainless Steel without External Barrier Layers Using Oxy-acetylene Flame," *Diamond Related Mater.* 7, 1043-1047 (1998).

Diamond Formation
C_2H_2/O_2
Stainless Steel
Substrate
Pretreatment

85346. Hahn, D.W., and K.F. McCarty, "Systematic Study of Diamond Film Deposition in an Atmospheric Pressure Stagnation Flow Flame Reactor," *Diamond Related Mater.* 7, 1320-1327 (1998).

Diamond Formation
$C_2H_2/H_2/O_2$
Strained Flames
N_2,Ar Effects
Growth Rates
Quality

85347. Wolden, C.A., C.E. Draper, Z. Sitar and J.T. Prater, "The Influence of Nitrogen Addition on the Morphology, Growth Rate and Raman Spectra of Combustion Grown Diamond," *Diamond Related Mater.* 7, 1178-1183 (1998).

Diamond Formation
$C_2H_2/O_2/N_2$
N_2 Effects
Growth Rates
Morphology

85348. Klein-Douwel, R.J.H., J.J. Schermer and J.J. ter Meulen, "CN Distribution in Flame Deposition of Diamond and Its Relation to the Growth Rate, Morphology and Nitrogen Incorporation of the Diamond Layer," *Diamond Related Mater.* 7, 1118-1132 (1998).

Diamond Formation
C_2H_2/O_2
CN 2-D LIF
N_2,C_2H_2 Purity
Effects

85349. Klein-Douwel, R.J.H., and J.J. ter Meulen, "Spatial Distributions of H, CN and C_2 in a Diamond Growing Oxyacetylene Flame," *Symp. (Int.) Combust. Proc.* 27, 2477-2483 (1998).

Diamond Formation
C_2H_2/O_2 Flame
CN,C_2,H Profiles
2-D LIF
Structure

85350. Yarina, K.L., D.S. Dandy, E. Jensen and J.E. Butler, "Growth of Diamond Films Using an Enclosed Methyl-Acetylene and Propadiene Combustion Flame," *Diamond Related Mater.* 7, 1491-1502 (1998).

Diamond Formation
MAPP Gas Flame
Growth Rates

85351. Horii, N., N. Suzuki, K.-i. Itoh, T. Kotaki and O. Matsumoto, "Deposition of Diamond from Plasma Jets with Chlorobenzenes as Carbon Source," *Diamond Related Mater.* 6, 1874-1882 (1997).

Diamond Formation
$Ar/H_2/$
$C_6H_{6-n}Cl_n$,n=1-3
DC Discharge
Cl Effects

85352. Ferreira, N.G., E.J. Corat, V.J. Trava-Airoldi, N.F. Leite and R.C.M. de Barros, "H Actinometry with CF_4 Addition in Microwave Plasma Assisted Chemical Vapor Deposition of Diamond," *Diamond Related Mater.* 6, 472-475 (1997).

Diamond Formation
$CF_4/H_2/Ar$
$CH_4/H_2/Ar$
Microwave Discharge
H_α Emission
O_2 Effects

85353. Hartmann, P., R. Haubner and B. Lux, "Deposition of Thick Diamond Films by Pulsed dc Glow Discharge CVD," *Diamond Related Mater.* 5, 850-856 (1996).

Diamond Formation
CH_4/H_2
Pulsed Discharge
High Deposition Rates

85354. Kuo, K.-P., and J. Asmussen, "An Experimental Study of High Pressure Synthesis of Diamond Films Using a Microwave Cavity Plasma Reactor," *Diamond Related Mater.* 6, 1097-1105 (1997).

Diamond Formation
CH_4/H_2
Microwave Discharge
High Pressure
Growth Rates

85355. Mutsukura, N., and K.-i. Yoshida, "Deposition of Diamond-Like Carbon Films in CH_4/Ne and CH_4/Kr Radiofrequency Plasmas," *Diamond Related Mater.* 6, 547-550 (1997).

Diamond Formation
CH_4/Ne,Kr
RF Discharge
Hardness
Properties

85356. Lindsay, J.W., J.M. Larson and S.L. Girshick, "Effect of Surface Species Concentrations and Temperature on Diamond Film Morphology in Inductively Coupled Radiofrequency Plasma CVD," *Diamond Related Mater.* 6, 481-485 (1997).

Diamond Formation
$CH_4/H_2/Ar$
RF Discharge
Morphology
Rates

85357. Ferreira, N.G., E.J. Corat, V.J. Trava-Airoldi and N.F. Leite, "Gas Phase Study with CF_4 and CCl_2F_2 Addition in Microwave CVD Diamond Growth," *Diamond Related Mater.* 7, 272-275 (1998).

Diamond Formation
$CH_4/H_2/O_2/M$
Microwave Discharge
$M=CF_4,CCl_2F_2$
Halogen Effects
Mass Analysis

85358. Ferreira, N.G., E.J. Corat, V.J. Trava-Airoldi, N.F. Leite and E. Del Bosco, "Evidence of Enhanced Atomic Hydrogen Production with Halogens in Diamond Microwave Plasma Assisted CVD," *Diamond Related Mater.* 7, 81-87 (1998).

Diamond Formation
$CH_4/H_2/CF_4$
$CH_4/H_2/CCl_2F_2$
Microwave Discharge
H-Atom
Enhancements

85359. Chatei, H., J. Bougdira, M. Remy, P. Alnot, C. Bruch and J.K. Kruger, "Combined Effect of Nitrogen and Pulsed Microwave Plasma on Diamond Growth," *Diamond Related Mater.* 6, 505-510 (1997).

Diamond Formation
CH_4/H_2
Microwave Discharge
Pulsed Mode
N_2 Effects

85360.	Chatei, H., J. Bougdira, M. Remy, P. Alnot, C. Bruch and J.K. Kruger, "Effect of Nitrogen Concentration on Plasma Reactivity and Diamond Growth in a $H_2/CH_4/N_2$ Microwave Discharge," *Diamond Related Mater.* 6, 107-119 (1997).	Diamond Formation $CH_4/H_2/N_2$ Microwave Discharge CH*,CN* Emission N_2 Effects
85361.	Mitsuda, Y., and S. Sakai, "Energy Distribution of H Atom and C_2 Radical during Diamond Growth in $H_2/Ar\text{-}CH_4\text{-}O_2$ Plasma," *Diamond Related Mater.* 6, 468-471 (1997).	Diamond Formation $CH_4/H_2/O_2/Ar$ Microwave Discharge H*,C_2* Emission Temperatures
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85363.	Tarr, J., and M. Kaufman, "Diamond Film Deposition from the Reaction of Hydrogen Atoms with Acetaldehyde," *Diamond Related Mater.* 7, 1328-1332 (1998).	Diamond Formation H_2/Ar Discharge CH_3CHO Addition CH_3 Role
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Laser Induced Nucleation

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Calculations
Data Comparison
Discrepancies

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Soot
Cavity Ringdown
LII
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Sizing
Phase Doppler
Laser Diffraction
Comparisons

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(See also Section 22 for Nucleation and Growth of Particles and Section 26 for Spectroscopy of Cluster Molecules)

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Nucleation

(85824) Measurements

IP(Ba_nO_m)
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C_n
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Raman Active
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(85711)	Reaction Dynamics, Mechanism	$C_{60} + O_3$
85394.	Weston, A., M. Murthy and S. Lalvani, "Synthesis of Fullerenes from Coal," *Fuel Processing Technol.* 45, 203-212 (1995).	Fullerene Formation Coal Arc Discharge Method
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(85836)	Collision Induced Dissociation Measurements	$D(Cu_n^+)$, n = 2-9
(85659)	Product OH Distributions, Cluster Effects	$H_2O.Ar(3\nu_{OH}) + h\nu$ $H_2O(3\nu_{OH}) + h\nu$
(85205)	Diffusion Coefficients, Cluster Effects	$H_2SO_4.nH_2O/N_2$ H_2SO_4/N_2
(85207)	Product Cluster Ions, Corona Discharge, Ambient Air	$H_3O^+(H_2O)_n$ $O_2^+(H_2O)$
(85792)	Structural Calculations, Geometries, Frequencies	$Li(H_2O)_n$ $Na(H_2O)_n$
(85793)	Dimer *cis/trans* Isomerization, Geometries, Frequencies, Structural Calculations	$(NO)_2$
(85795)	Structural Calculations, Geometries, Infrared Spectra, Energies	$Na(H_2O)_n^-$
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(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

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CCl_4, $SiCl_4$
$GeCl_4$
9-25 eV Excited
Fragment
Fluorescence
Spectra

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ClCHO(A-X)
Cavity Ringdown
Spectrum
Assignments
Constants

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HCO(B-X)
LIF Spectrum
v Energy Levels
Assignments
Dipole Moments

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HCHS(A-X)
OODR/Fluorescence
Spectra
Rotational
Relaxation
Perturbations

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CH_3O(X)
Jahn-Teller Effect
Vibronic
Analysis

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OCS
Absorption
Cross Sections
200-260 nm
170-370 K

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CO_2
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13,000 Line
v,J Energy Hamiltonian

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CO_2, C_2H_2
Weak Combination
Line Absorption
Cavity Ringdown
Lineshapes
Wavelengths

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$CS_2^{\pm}$,$C_2S_4^+$
FTIR Spectra
Assignments
Frequencies
Matrix Study

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$C_2H_2(S_1\text{-}S_0)$
LIF Spectral
Interpretation
IVR

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$C_2H_2F_4$,$C_2H_3F_3$
IR Absorption
Cross Sections
Erratum

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CH_3CFCl_2
CH_3CF_2Cl
(3-5)ν_{CH} Overtone
Optoacoustic
Spectra

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C_2H_5Br
VUV Absorption
Spectrum
Assignments
Oscillator
Strengths

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C_2H_5S(A,X)
2-Photon PFI-PE
Spectra
A/X Energy Splitting
IPS

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C_3^-(C,B,A-X)
C_3^-(b-X)
Absorption Spectra
Matrix Study
Gas Phase
Photodetachment
Spectral Constants
Measurements

(85620) LIF Spectra, Measurements

n-,*i*-C_3H_7O

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c-$C_4HN_2Cl_3$
c-$C_4H_2N_2Cl_2$
IR,Raman
Spectra
Constants
Geometries

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(85214)	Photoionization Cross Sections, Measurements	ClO,ClO_2
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CuCN,AgCN
EAs,Frequencies
Anion PES Spectra
Structures

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CuNO,$CuNO^+$
$Cu(NO)_2$,$Cu(NO)_2^-$
FTIR Spectra
Assignments
Matrix Study

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FO
Rotational
Spectrum
Constants
r_0

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FeH(C,b)
LIF Spectra
Low-lying
Electronic State
Assignments

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GaN,GaN_2,InN_2
MN_3,M_3N
FTIR Spectra
Assignments
M=Ga,In,Tl
Matrix Study

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GeH^+(A-X)
Photodissociation
Spectra
Fragment Ions

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GeS(A-X)
Emission Spectrum
Isotopes
Constants
F.C. Factors
r-Centroids

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H(2S-1S)
Frequency
Measurement

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$H^{79}Br$,$H^{81}Br$
IR Spectrum
Line Parameters
Measurements

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HCl
Photoionization
Spectrum
Calculations

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HI
IR,Far IR Spectra
Line Parameters

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HNCO(S_1)
Spectral Origin
Frequencies
Multiphoton
Fluorescence
Photofragment
Analyses

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HNO_3
IR Spectrum
HITRAN Database
Lines
Cross Sections

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HOF^-
Photodetachment
Spectrum
HOF P.E. Surface
Resonances
Calculations

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HONO
IR Absorption
Cross Sections
Band Strengths

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H_2
(1+2′) MPI
Autoionization
Photoelectron
Energy Spectrum

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HOD($5\nu_{OD}$)
Overtone
Absorption
Spectrum
FT Intracavity
Constants

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H_2O
720-1400 cm^{-1}
Lines,Assignments

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H_2O
Absorption
1540-2170 cm^{-1}
Nonlinear
IR Laser Generation

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H_2S
Absorption
Cross Sections
160-260 nm
170-370 K

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IBr
2-Photon,1-Color
ZEKE-PFI
Spectrum
Neutral/Ion
Constants
IP($X^2\Pi_{1/2,3/2}$)

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ICl(β-A)
Electric
Dipole Moment
OODR Spectrum

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KRb(A-X)
LIF Spectrum
Ground State
Dunham Constants
P.E. Curve
D_e(X)

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LaO(B-X)
LIF Spectrum
Constants

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LnH,LnH_2
LnH_3,LnH_4
FTIR Spectra
Assignments
Ln=Ce,Pr,Sm
Eu,Gd,Tb
Matrix Study

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NLnO
FTIR Spectra
Ln=Lanthanide
Assignments
Frequencies
Matrix Study

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Li_3,Na_3(A-X)
2-Color
REMPI Spectra
Mass Detector

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$M(CO)_n$,$M(CO)_n^\pm$
M=Ni,Pd,Pt
FTIR Spectra
Assignments
Frequencies

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MC_3^-
PES Spectra
M=Sc thru Ni
EA(MC_3)
Frequencies
Structures

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$M(NO)_n$,MNO^+
$M(NO)_n^-$
M=Fe,Co,Ni
FTIR Spectra
Assignments
Frequencies

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MO_2,MO_2^-
MO_3,MO_4
M=Re,Ru,Os
FTIR Spectra
Frequencies
Matrix Study

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MoO($^3\Delta$-X)
WO(B,A-X)
Absorption
Spectral Bands

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NCl
REMPI Spectra
Assignments
Three $^1\Sigma$ States

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NO(X$^2\Pi$)
Rotational
Spectrum
Isotopes
Constants

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NO,5.3 μm
HITRAN Database
Critical Review

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NO
Rydberg States
4-Wave Mixing
ASE Role

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NO_2 ,SO_2
IR Spectra
HITRAN Database
Line Parameters

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NO_2
231-794 nm
Absorption
Cross Sections
221-293 K

85472. Biesheuvel, C.A., J. Bulthuis, M.H.M. Janssen, S. Stolte and J.G. Snijders, "High Resolution Laser Spectroscopy of NO_2 Just above the (X^2A_1-A^2B_2) Conical Intersection: Transitions of K_=1 Stacks," *J. Chem. Phys.* 112, 3633-3642 (2000).
NO_2(A-X)
Absorption
High Resolution
10000-14000 cm^{-1}
Level Energies
Analysis

(85515) Predissociation Spectrum, Constants, Measurements
N_2(b),v=1

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N_2H_4
$N_2H_3(CH_3)$
Absorption
Cross Sections
Diode Laser

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Absorption
NaH(A-X)
Cavity Ringdown
Transition
Moment
Measurements

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$Na_3(2^4E'-1^4A_2')$
LIF
He Nanodroplet
Assignments
Frequencies

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$OH+CH_4$
Transition State
IR Spectra
Lifetimes
Dynamics

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$^{16,16,17}O_3$
$^{16,17,16}O_3$
IR Spectral
Parameters

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O_3
$2\nu_2$, $3\nu_2-\nu_2$ Bands
IR Spectra
Constants
Band Intensities

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O_3
Absorption
Cross Sections
202-293 K
231-794 nm

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$(O_2(a))_2/(O_2)_2$
Collision Induced
Absorption
Cross Sections
$O_2(a),v=0,1$
Transitions
Band Intensities

85481.	Biennier, L., D. Romanini, A. Kachanov, A. Campargue, B. Bussery-Honvault and R. Bacis, "Structure and Rovibrational Analysis of the $[O_2(^1\Delta_g)_{v=0}]_2 \leftarrow [O_2(^3\Sigma_g^-)_{v=0}]_2$ Transition of the O_2 Dimer," *J. Chem. Phys.* 112, 6309-6321 (2000).	$(O_2(a))_2/(O_2)_2$ Absorption Spectrum Cavity Ringdown Assignments Constants
85482.	Bauschlicher Jr., C.W., M. Zhou and L. Andrews, "A Study of the Products of the Reaction of Phosphorus and Dioxygen," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3566-3571 (2000).	PO_2, PO_2^- PO_3, PO_3^- P_2O, P_2O_3, P_4 FTIR Spectra Frequencies P(s) Ablation/O_2 Matrix Study
85483.	Archer, C.P., J.M.F. Elks and C.M. Western, "The $C^3\Pi$, $d^1\Pi$ and $e^1\Pi$ States of SO," *J. Chem. Phys.* 112, 6293-6300 (2000).	SO(e,d,C-X) (1+1) MPI Spectra Assignments d-State P.E. Curve
85484.	Iachello, F., F. Perez-Bernal, T. Muller and P.H. Vaccaro, "A Quantitative Study of Non-Condon Effects in the $S_2O(C\rightarrow X)$ Emission Spectrum," *J. Chem. Phys.* 112, 6507-6510 (2000).	S_2O(C-X) Emission Spectrum Intensities
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(85595)	$SiCl_4/O_2$ Combustion, Matrix Isolation Method	$SiOCl_2$ IR Spectrum
(85845)	Photoionization Spectrum, IP, Calculations	Si_2
85486.	Polo, A.M., J.M.L. Poyato, J.J. Camacho and A. Pardo, "Intensity Study of LIF Spectrum for the $(B0_u^+ \rightarrow X0_g^+)$ System of a Tellurium Natural Sample," *J. Quant. Spectrosc. Radiat. Transfer* 60, 989-1000 (1998).	Te_2(B-X) LIF Spectra Ar^+ Laser Induced Natural Isotopes Measurements Radiative Lifetime Calculations
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V_2
Electronic
Spectral
Assignment
Calculations

85489. Hansford, G.M., M. Lorono and P.B. Davies, "Infrared Laser Jet Spectroscopy of the ν_6 Fundamental Band of $W(CO)_6$: Rotational Structure and Octahedral Splitting," *J. Chem. Phys.* 112, 3620-3626 (2000).

$W(CO)_6$, ν_6
IR Absorption
Cooled Beam
Spectral Constants

27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

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$Ag^+(4d^95p)$
Lifetimes
Transition
Probabilities
Calculations

(85756) Lifetime, P.E. Curves, Low-lying States, Spectral Constants, Calculations — AlS(B)

85491. Wouters, M.J., M. Khachan, I.S. Falconer and B.W. James, "Quenching of Excited Ar and H by H_2 in a Gas Discharge," *J. Phys. B. At. Mol. Opt. Phys.* 32, 2869-2880 (1999).

$Ar(4p') + H_2$
$H(n=4,5) + H_2$
Quenching
Cross Sections
Measurements

(85208) Chemi-ionization, Electronic State Role, Measurements — $BaO^* + H$

(85817) Rotational Relaxation Rate Constants, Propensities, Measurements — $CN(A,v=3,N=60) + Ar$

85492. Chen, Y., and M.C. Heaven, "Comparison of Direct and Resonant Scattering for H_2+$CN(A^2\Pi)$: Collisional Energy Transfer versus Predissociation of $CN(A)$-H_2 Complexes," *J. Chem. Phys.* 112, 7416-7424 (2000).

$CN(A) + H_2$
Quenching
Energy Transfer
ortho/para Effects
Spectral
Measurements

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$CO(a,v=3,J)$
Metastable
Lifetime
Measurements

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CO_2^-
Metastable States
Lifetimes
Identities

(85610) Rate Constant Measurements — $C_2(a) + NO$

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CCH(B)
Fluorescence
Predissociative
Lifetimes
D_0''

(85647) Predissociative Lifetimes, Pump/Probe Method

C_2H_2
Rydberg States

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$CH_3CHO(S_1/T_1)$
$CD_3CDO(S_1/T_1)$
Fluorescence
Decays
State Interactions
Lifetimes

(85801) Electronic Relaxations, fs Pump/Probe Measurements

c-$C_4H_4N_2(S_2, S_1)$

(85428) Lifetime, S_1/S_0 Internal Conversion, Cavity Ringdown Absorption Spectrum, Jet Cooled, Conical Intersection

$C_{10}H_8(S_1)$

85497. Salazar, M.G., J.M.O. Rocha, A.G. Urena and G. Roberts, "Collisional Dynamics of $Ca(^1D)+HBr$ Reactions: Evidence for Transition State Motions," *Mol. Phys.* 97, 967-976 (1999).

$Ca(^1D)+HBr$
Cross Sections
CaBr(B,A) Products
Energy Dependences
Dynamics

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$Cd(^3P_J)+Cd,Ne$
Mixing
Cross Sections
Diffusion
Coefficients

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$Cl(^2P_{1/2})+M$
M = 15 Molecules
Cl + HBr,DBr
$I(^2P_{1/2})+ICl$
Rate Constant
Measurements

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Cross Sections
Measurements

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Spectral Constants

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(85766)	P.E. Surfaces, NH_2(A), Correlations, Energies	$N(^2D) + H_2$ NH(a) + H
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Cross Sections

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Measurements

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Rate Constants
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Quenching
Rate Constants
v,J Relaxation
CH_4/O_2 Flame
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$O_2(a)+H_2,O_2$
$O_2(a)$/Quartz
Quenching
Rate Constant
Measurements

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PO(X,v,J)

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He,N_2,O_2,O_3

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Radiative
Lifetimes
F.C. Factors
Spectral Constants
Calculations

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Strength
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CO

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(85768)	F.C. Factor Calculations, P.E. Curves, Spectral Constants	NaO^+(b-a,A-X)
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(85418)	Lineshapes, Cavity Ringdown Absorption Measurements	CO_2,C_2H_2 Combination Bands
(85566)	Lineshapes, Diode Laser Absorption, Combination Bands	CO_2,H_2O NH_3,N_2O

(85781) Infrared Intensities, Frequencies, Structural Calculations | $CH_3C(O)OO$ $CH_3C(O)OONO_2$

(85782) Infrared Intensities, Structural Calculations, Geometries, Frequencies | $C_2O(A,X)$

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(85480) Band Intensities, ($v'=1,0-v''=0,0$) and ($v'=0,0-v''=0,0$) Transitions, Measurements | $(O_2(a))_2/(O_2)_2$

(85478) Band Intensities, Infrared Spectra, Constants | $O_3(2\nu_2,3\nu_2-\nu_2)$

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(See also Section 32 for 2-D Mapping Measurements)

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85572.	McNesby, K.L., R.R. Skaggs, A.W. Miziolek, M. Clay, S.H. Hoke and C.S. Miser, "Diode Laser Based Measurements of Hydrogen Fluoride Gas during Chemical Suppression of Fires," *Appl. Phys. B. Laser Opt.* 67, 443-447 (1998).	Absorption HF Diode Laser Halon Alternative Fire Suppression Measurements
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(85452)	Difference-Frequency Infrared Nonlinear Laser Generation, 1540-2170 cm^{-1}, Method	Absorption H_2O
85574.	Ehret, G., A. Fix, V. Weiss, G. Poberaj and T. Baumert, "Diode Laser Seeded Optical Parametric Oscillator for Airborne Water Vapor DIAL Application in the Upper Troposphere and Lower Stratosphere," *Appl. Phys. B. Laser Opt.* 67, 427-431 (1998).	DIAL H_2O OPO Laser Method
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(85386) Soot Volume Fraction Measurements, CH_4/Air, Comparisons — Cavity Ringdown; LII Methods

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85584. Gottwald, U., and P. Monkhouse, "Single-Port Optical Access for Spectroscopic Measurements in Industrial Flue Gas Ducts," *Appl. Phys. B. Laser Opt.* 69, 151-154 (1999). — Fragmentation; LIF; Alkali Species; Flue Gases; High Pressure; Measuring Port

85585. Bombach, R., and B. Kappeli, "Simultaneous Visualization of Transient Species in Flames by Planar Laser Induced Fluorescence Using a Single Laser System," *Appl. Phys. B. Laser Opt.* 68, 251-255 (1999). — PLIF; CH,CN,HCHO; CH_4/Air Flame; Simultaneous; Dye Laser System

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(85202)	Arcjet Measurements	2-Photon LIF N-Atom
85590.	Schulz, C., V. Sick, U.E. Meier, J. Heinze and W. Stricker, "Quantification of NO(A-X), (0,2) Laser Induced Fluorescence: Investigation of Calibration and Collisional Influences in High Pressure Flames," *Appl. Opt.* 38, 1434-1443 (1999).	LIF NO(A-X),(0,2) CH_4,C_7H_{16}/Air Calibration Processes
85591.	Yang, S.-R., J.-R. Zhao, C.-J. Sung and G. Yu, "Multiplex CARS Measurements in Supersonic H_2/Air Combustion," *Appl. Phys. B. Laser Opt.* 68, 257-265 (1999).	CARS T,H_2,O_2 Multiplexed Measurements H_2 Supersonic Combustor
85592.	Farrow, R.L., and D.J. Rakestraw, "Analysis of Degenerate Four-Wave Mixing Spectra of NO in a $CH_4/N_2/O_2$ Flame," *Appl. Phys. B. Laser Opt.* 68, 741-747 (1999).	DFWM NO(A-X) $CH_4/O_2/N_2$ Flame Detection Limit
85593.	Latzel, H., A. Dreizler, T. Dreier, J. Heinze, M. Dillmann, W. Stricker, G.M. Lloyd and P. Ewart, "Thermal Grating and Broadband Degenerate Four-Wave Mixing Spectroscopy of OH in High Pressure Flames," *Appl. Phys. B. Laser Opt.* 67, 667-673 (1998).	DFWM OH(A-X) CH_4/Air Flames

31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

(85546)	Mass Analysis, C_3H_6/O_2/Ar Flame, Perturbation Analysis, Temperature Changes	Probe Sampling Profiles
(85585)	CH_4/Air Flame, PLIF, Simultaneous Dye Laser Measurements	Species Profiles CH,CN,HCHO
85594.	McEnally, C.S., and L.D. Pfefferle, "Experimental Study of Nonfuel Hydrocarbons and Soot in Coflowing Partially Premixed Ethylene/Air Flames," *Combust. Flame* 121, 575-592 (2000).	Species Profiles C_1-C_{12} Hydrocarbons PAHS,Soot C_2H_4 Flames Premixed Effects

85595.	Junker, M., A. Wilkening, M. Binnewies and H. Schnockel, "The Detection of $O{=}SiCl_2$ as an Intermediate during the Combustion Process of $SiCl_4$ with O_2," *Eur. J. Inorg. Chem* 1531-1535 (1999).	$SiOCl_2$ Intermediate Identified IR Spectrum $SiCl_4/O_2$ Combustion

32. MAPPING/TOMOGRAPHIC METHODS

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(85585)	CH_4/Air Flame, Simultaneous Dye Laser Measurements	PLIF CH,CN,HCHO
(85185)	Turbulent $CH_4/H_2/N_2$ Diffusion Flame, Raman, Rayleigh Single Pulse Measurements	PLIF,CH,NO,OH
(85184)	Turbulent CH_4 Jet Flame, Structure, Simultaneous Measurements	PLIF,CH,OH
(85200)	2-D Mapping, $CH_3I+h\nu$, REMPI Monitor	$CH_3(v),I(^2P_{1/2,3/2})$ Velocities
(85348)	Diamond Formation, C_2H_2/O_2 Flame, N_2, C_2H_2 Purity Effects	PLIF,CN
(85349)	Diamond Formation, C_2H_2/O_2 Flame, Profiles, Structure	PLIF,CN,C_2,H
85597.	Kirby, B.J., and R.K. Hanson, "Planar Laser Induced Fluorescence Imaging of Carbon Monoxide Using Vibrational (Infrared) Transitions," *Appl. Phys. B. Laser Opt.* 69, 505-507 (1999).	2-D Imaging CO,IR LIF 2ν Pumping
85598.	Tichy, F.E., T. Bjorge, B.F. Magnussen, P.E. Bengtsson and F. Mauss, "Two-Dimensional Imaging of Glyoxal, $(CHO)_2$, in Acetylene Flames Using Laser Induced Fluorescence," *Appl. Phys. B. Laser Opt.* 66, 115-119 (1998).	2-D LIF $(CHO)_2$ Turbulent C_2H_2 Flames
(85335)	Volume Fractions, C_2H_4/Air Flame, Radial Profiles	2-D Imaging Soot
(85271)	I.C. Engine, C_3H_8 Fueled, Ultraviolet Absorption Corrections	PLIF,NO
(85187)	Turbulent CH_4/Air Flame, High Speed Imaging	PLIF,OH

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

85599.	Schafer, S., M. Mashni, J. Sneider, A. Miklos, P. Hess, H. Pitz, K.-U. Pleban and V. Ebert, "Sensitive Detection of Methane with a 1.65 μm Diode Laser by Photoacoustic and Absorption Spectroscopy," *Appl. Phys. B. Laser Opt.* 66, 511-516 (1998).	Optoacoustic Absorption CH_4 Diode Laser Monitoring Methods
(85739)	Optoacoustic Absorption, IR OPO Narrowline Tunable Laser	CH_4
(85422)	(3-5)ν_{CH} Overtone Spectra, Optoacoustic Monitor	CH_3CFCl_2 CH_3CF_2Cl
(85568)	CO_2 Laser Absorption Coincidences, Pressure Effects, Optoacoustic Detection	C_2H_4, NH_3
(85815)	Relaxation Rates, Optoacoustic Measurements	$SF_6(v)+Ar$

34. FLAME KINETIC MODELING

85600.	Ferrendier, M., P. Duchene and A. Trouve, "Reduced Chemical Kinetic Mechanisms for Combustion," *Combustion* 1, 21-79 (1999).	Kinetic Modeling Flames Reduced Scheme Methods Review
(85152)	Kinetic Modeling, Ignition Delays	$N_2H_3(CH_3)/O_2/Ar$
85601.	Korobeinichev, O.P., S.B. Ilyin, T.A. Bolshova, V.M. Shvartsberg and A.A. Chernov, "The Chemistry of the Destruction of Organophosphorus Compounds in Flames. III. The Destruction of Dimethyl Methyl Phosphonate and Trimethyl Phosphate in a Flame of Hydrogen and Oxygen," *Combust. Flame* 121, 593-609 (2000).	Phosphorus Flame Chemistry Species Profiles Kinetic Modeling
(85149)	Kinetic Modeling, Reaction Paths, Self-ignition	SiH_4/O_2

35. PYROLYSIS KINETICS/STUDIES

(See also Section 4 for Coal and Waste Pyrolysis)

(85331)	Shock Tube Pyrolysis, Soot Formation, Growth Rates	CCl_4/Ar $CCl_4/Fe(CO)_5/Ar$ $CCl_4/H_2/Ar$
85602.	Murphy, D.B., R.W. Carroll and J.E. Klonowski, "Analysis of Products of High Temperature Pyrolysis of Various Hydrocarbons," *Carbon* 35, 1819-1823 (1997).	Pyrolysis CH_4, C_2H_6, C_3H_8 C_2H_2, C_2H_4, *neo*-C_5H_{12} Aromatic Products C_2H_2 Role

(85034) Liquefaction/Gasification, Product Yields — Pyrolysis; Natural Gas

85603. Bohm, H., and H. Jander, "PAH Formation in Acetylene/Benzene Pyrolysis," *Phys. Chem. Chem. Phys.* 1, 3775-3781 (1999). — Pyrolysis; C_2H_2/C_6H_6; PAH Formation; Shock Tube

(85328) Carbon Microcoils Formation, Ni Catalyzed Method — C_3H_8 Pyrolysis

85604. Sendt, K., G.B. Bacskay and J.C. Mackie, "Pyrolysis of Furan: Ab Initio Quantum Chemical and Kinetic Modeling Studies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1861-1875 (2000). — Pyrolysis; *c*-C_4H_4O; Mechanism; Kinetic Modeling

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

85605. Simos, T.E., "An Exponentially Fitted Runge-Kutta Method for the Numerical Integration of Initial-Value Problems with Periodic or Oscillating Solutions," *Comput. Phys. Commun.* 115, 1-8 (1998). — Runge-Kutta; Integration; Method; Oscillatory Solutions

(85278) Reaction Time Constant Concepts — Tropospheric; Kinetic Modeling

85606. Orlando, J.J., and J.B. Burkholder, "Identification of BrONO as the Major Product in the Gas Phase Reaction of Br with NO_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2048-2053 (2000). — BrONO+Br; $BrNO_2$+Br; Rate Constants; Br+NO_2+M; BrONO Product; Isomerization

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(85646) Rate Constant Assessment, $CF_3COF+h\nu$ Measurements — CF_3+FCO(+M)

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85609. Louis, F., D.R. Burgess Jr., M.-T. Rayez and J.-P. Sawerysyn, "Kinetic Study of the Reactions of CF_3O_2 Radicals with Cl and NO," *Phys. Chem. Chem. Phys.* 1, 5087-5096 (1999).

CF_3O_2+Cl
CF_3O_2+NO
Rate Constants
Channels

85610. Geiger, H., P. Weisen and K.H. Becker, "A Product Study of the Reaction of CH Radicals with Nitric Oxide at 298 K," *Phys. Chem. Chem. Phys.* 1, 5601-5606 (1999).

CH+NO
CN,NH,NCO+NO
C_2(a)+NO
Rate Constant Measurements
Reaction Channels

85611. Ziemer, H., S. Dobe, H.G. Wagner, M. Olzmann, B. Viskolcz and F. Temps, "Kinetics of the Reactions of HCO with H and D Atoms," *Ber. Bunsenges. Phys. Chem.* 102, 897-905 (1998).

HCO+H,D
Rate Constants
Measurements

85612. Deters, R., M. Otting, H.G. Wagner, F. Temps and S. Dobe, "Rate Constant for the Reaction $CH_3+CH_2(X^3B_1)$ at 298 K," *Ber. Bunsenges. Phys. Chem.* 102, 978-981 (1998).

CH_2+CH_3
CH_3+CH_3+M
Rate Constant
Measurements

85613. You, Y.-Y., and N.S. Wang, "Rate Coefficients of the Reactions of CN and NCO with O_2 and NO_2 at 296 K," *J. Chinese Chem. Soc.* 40, 337-343 (1993).

CN+NO_2,O_2
NCO+NO_2,O_2
Rate Constants
Measurements

85614. Tichenor, L.B., J.L. Graham, T. Yamada, P.H. Taylor, J. Peng, X. Hu and P. Marshall, "Kinetic and Modeling Studies of the Reaction of Hydroxyl Radicals with Tetrachloroethylene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1700-1707 (2000).

C_2Cl_4+OH
Rate Constants
T Dependence
Mechanisms

85615. Schneider, W.F., T.J. Wallington, J.R. Barker and E.A. Stahlberg, "CF_3CFHO Radical: Decomposition vs. Reaction with O_2," *Ber. Bunsenges. Phys. Chem.* 102, 1850-1856 (1998).

$CF_3CFHO+O_2$
$CF_3CFHO\rightarrow$
Rate Constants
Enigma Resolution

85616. Mashino, M., M. Kawasaki, T.J. Wallington and M.D. Hurley, "Atmospheric Degradation of $CF_3OCF=CF_2$: Kinetics and Mechanism of Its Reaction with OH Radicals and Cl Atoms," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2925-2930 (2000).

$CF_3OC_2F_3$+Cl
$CF_3OC_2F_3$+OH
Rate Constants
Product Yields

85617. DeSain, J.D., P.Y. Hung, R.I. Thompson, G.P. Glass, G. Scuseria and R.F. Curl, "Kinetics of the Reaction of Propargyl Radical with Nitric Oxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3356-3363 (2000).

C_3H_3+NO(+He)
Rate Constants
P,T Dependence

85618. Seetula, J.A., "Kinetics and Thermochemistry of the $C_3H_5+HBr\rightleftarrows C_3H_6+Br$ Equilibrium," *Phys. Chem. Chem. Phys.* 1, 4727-4731 (1999).

C_3H_5+HBr
Rate Constants
$\Delta H_f(C_3H_5)$
Assessments

85619. Wollenhaupt, M., S.A. Carl, A. Horowitz and J.N. Crowley, "Rate Coefficients for Reaction of OH with Acetone between 202 and 395 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2695-2705 (2000).

$(CH_3)_2CO + OH$
Rate Constants
T Dependence
Arrhenius
Curvature
Measurements

85620. Mund, C., C. Fockenberg and R. Zellner, "LIF Spectra of *n*-Propoxy and *i*-Propoxy Radicals and Kinetics of their Reactions with O_2 and NO_2," *Ber. Bunsenges. Phys. Chem.* 102, 709-715 (1998); *Phys. Chem. Chem. Phys.* 1, 2037 (1999).

$n\text{-}C_3H_7O + NO_2, O_2$
$i\text{-}C_3H_7O + NO_2, O_2$
Rate Constants
P,T Dependences
LIF Spectra

(85604) Kinetic Modeling, Mechanism

$c\text{-}C_4H_4O$
Pyrolysis

85621. Hein, H., A. Hoffmann and R. Zellner, "Direct Investigations of Reactions of 2-Butoxy Radicals Using Laser Pulse Initiated Oxidation: Reaction with O_2 and Unimolecular Decomposition at 293 K and 50 mbar," *Ber. Bunsenges. Phys. Chem.* 102, 1840-1849 (1998).

$C_4H_9O + O_2$
$C_4H_9O \rightarrow$
Rate Constants

85622. Hein, H., A. Hoffmann and R. Zellner, "Direct Investigations of Reactions of 1-Butoxy and 1-Pentoxy Radicals Using Laser Pulse Initiated Oxidation: Reaction with O_2 and Isomerization at 293 K and 50 mbar," *Phys. Chem. Chem. Phys.* 1, 3743-3752 (1999).

$C_4H_9O + O_2$
$C_4H_9O \rightarrow$
$C_5H_{11}O + O_2$
$C_5H_{11}O \rightarrow$
Rate Constants
Measurements

85623. Aschmann, S.M., J. Arey and R. Atkinson, "Atmospheric Chemistry of Selected Hydroxycarbonyls," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3998-4003 (2000).

$RCOR'OH + NO_3$
$RCOR'OH + OH, O_3$
Rate Constants
6 Hydroxycarbonyls

85624. Bohn, B., and C. Zetzsch, "Gas Phase Reaction of the OH-Benzene Adduct with O_2: Reversibility and Secondary Formation of HO_2," *Phys. Chem. Chem. Phys.* 1, 5097-5107 (1999).

$C_6H_6 + OH$
$C_6H_6.OH + NO, O_2$
$C_6H_6.OH + H_2O_2$
Rate Constants
Measurements

(85499) Rate Constants, Measurements

$Cl + HBr, DBr$

(85519) Rate Constants, Measurements

$Cl + N_2O$
$F + N_2O$

85625. Knight, G.P., T. Beiderhase, F. Helleis, K. Moortgat and J.N. Crowley, "Reaction of HO_2 with ClO: Flow Tube Studies of Kinetics and Product Formation between 215 and 298 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1674-1685 (2000).

$ClO + HO_2$
Rate Constants
T Dependence
HOCl Product

85626. Skodje, R.T., D. Skouteris, D.E. Manolopoulos, S.-H. Lee, F. Dong and K. Liu, "Observation of a Transition State Resonance in the Integral Cross Section of the F+HD Reaction," *J. Chem. Phys.* 112, 4536-4552 (2000).

F+HD
Cross Beam
Cross Sections
Branching Ratio
Reaction Dynamics

85627. Becerra, R., and R. Walsh, "A Gas Phase Kinetic Study of the Reaction of Germylene with Trimethylsilane: Absolute Rate Constants, Temperature Dependence and Mechanism," *Phys. Chem. Chem. Phys.* 1, 5301-5304 (1999).

$GeH_2+SiH(CH_3)_3$
Rate Constants
T,P Dependences
Mechanism

85628. Campbell, M.L., "Temperature Dependent Rate Constants for the Reactions of Gas Phase Lanthanides with CO_2," *Phys. Chem. Chem. Phys.* 1, 3731-3735 (1999).

$Ln+CO_2$
Rate Constants
$Ln=La \rightarrow Yb$
T Dependences

85629. Becker, K.H., H. Geiger, F. Schmidt and P. Wiesen, "Kinetic Investigation of NCO Radicals Reacting with Selected Hydrocarbons," *Phys. Chem. Chem. Phys.* 1, 5305-5309 (1999).

$NCO+C_2H_6$
$NCO+C_3H_4,C_3H_6$
$NCO+C_4H_6,C_4H_8$
Rate Constants
Measurements

85630. Deppe, J., G. Friedrichs, A. Ibrahim, H.-J. Romming and H.G. Wagner, "The Thermal Decomposition of NH_2 and NH Radicals," *Ber. Bunsenges. Phys. Chem.* 102, 1474-1485 (1998).

$NH+M$
NH_2+M
Rate Constants
T Dependences
Channels

85631. Canosa-Mas, C.E., S. Carr, M.D. King, D.E. Shallcross, K.C. Thompson and R.P. Wayne, "A Kinetic Study of the Reactions of NO_3 with Methyl Vinyl Ketone, Methacrolein, Acrolein, Methyl Acrylate and Methyl Methacrylate," *Phys. Chem. Chem. Phys.* 1, 4195-4202 (1999).

$NO_3+CH_3COC_2H_3$
$NO_3+CH_2C(CH_3)CHO$
$NO_3+C_2H_3CHO$
$NO_3+C_2H_3COOCH_3$
$NO_3+CH_2C(CH_3)COOCH_3$
Rate Constants

85632. Berndt, T., I. Kind and H.-J. Karbach, "Kinetics of the Gas Phase Reaction of NO_3 Radicals with 1-Butene, *trans*-Butene, 2-Methyl-2-butene and 2,3-Dimethyl-2-butene Using LIF Detection," *Ber. Bunsenges. Phys. Chem.* 102, 1486-1491 (1998).

$NO_3+C_4H_8$
$NO_3+C_5H_{10},C_6H_{12}$
Rate Constant
Measurements

85633. Cox, R.M., and J.M.C. Plane, "An Experimental and Theoretical Study of the Reactions $NaO+H_2O(D_2O) \rightarrow NaOH(D)+OH(OD)$," *Phys. Chem. Chem. Phys.* 1, 4713-4720 (1999).

$NaO+H_2O$
$NaO+D_2O$
Rate Constants
T Dependences
Measurements

85634. Becker, K.H., C.M.F. Dinis, H. Geiger and P. Wiesen, "The Reactions of OH Radicals with Di-*i*-Propoxymethane and Di-*sec*-Butoxymethane: Kinetic Measurements and Structure Activity Relationships," *Phys. Chem. Chem. Phys.* 1, 4721-4726 (1999).

$OH+(C_3H_7O)_2CH_2$
$OH+(C_4H_9O)_2CH_2$
Rate Constants

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$OH+O_3$
HO_2+O_3
Rate Constants
O_3/O_2
OH Catalyzed
Conversion Cycle
T Dependence

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$Si+SiCl_4$
Rate Constant
T Independent
Shock Tube
Measurement

85637. Srinivasan, J., and D.G. Truhlar, "Comment on Rate Constants for Reactions of Tritium Atoms with H_2, D_2 and HD," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1965-1967 (2000).

$T+H_2,HD,D_2$
Rate Constants
Comment

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

85638. Ivanenko, M.M., H. Handreck, J. Gothel, W.Fuss, K.-L. Kompa, P. Hering, "Isotope-Selective Infrared Multiphoton Dissociation of $CHClF_2$ in the Presence of NO_2," *Appl. Phys. B. Laser Opt.* 65, 577-582 (1997).

IR MPD
$CHClF_2/NO_2/He$
Product COF_2
Isotopic
Enrichment

(85200) $CH_3(v)$, $I(^2P_{1/2,3/2})$ Product Velocity Mapping, REMPI Monitor

$CH_3I+h\nu$

85639. Thomas, S.L., V.Y. Young and S. Hoke, "Photochemical Hydrogen Iodide Gas Generation from Iodomethane and 2-Iodopropane," *J. Photochem. Photobiol. A. Chem.* 114, 167-171 (1998).

$CH_3I+h\nu$
$C_3H_7I+h\nu$
Product HI
Quantum Yields

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$CH_3OH,CH_3OD+h\nu$
$CD_3OH+h\nu$
$CH_3CD_2CH_3+h\nu$
$C_2H_4,CH_3CCH+h\nu$
Product H,H_2
Channels
Dynamics

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$CH_4+h\nu$
Kinetic Modeling
Data Fitting
Current
Inadequacies

85642. Maul, C., and K.-H. Gericke, "Aspects of Photoinduced Molecular Three-Body Decay," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2531-2541 (2000).

$COCl_2$,COFCl,$SOCl_2$
ABC+hν
3 Product Channel
Review

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CS_2+hν
S_2 Yields
Magnetic Effects

85644. Ma, P.H., B. Wu and R.W. Carr, "Isotopically Selective Infrared Multiphoton Dissociation of 2-Chloro-1,1,1-trifluoroethane: ^{13}C Selectivity and Mechanism," *Appl. Phys. B. Laser Opt.* 68, 107-110 (1999).

IR MPD
CF_3CH_2Cl
Major Products
^{13}C Isotopic
Selectivity

85645. Malanca, F.E., G.A. Arguello, E.H. Staricco and R.P. Wayne, "The Photolysis of CF_3COCl in the Presence of O_2 and CO: Catalytic Oxidation of CO to CO_2 and the Formation of Polyoxygenated Intermediates," *J. Photochem. Photobiol. A. Chem.* 117, 163-169 (1998).

CF_3COCl+hν
Dynamics
CF_3O+CO
CF_3OCO+O_2
Mechanism

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CF_3COF+hν
Products
c-C_6H_{12},O_2
Additive Effects
Quantum Yields
CF_3+FCO(+M)
Rate Constant

85647. Sorensen, S.L., O. Bjorneholm, I. Hjelte, T. Kihlgren, G. Ohrwall, S. Sundin, S. Svensson, S. Buil, D. Descamps, A. L'Huillier, J. Norin and C.-G. Wahlstrom, "Femtosecond Pump-Probe Photoelectron Spectroscopy of Predissociative Rydberg States in Acetylene," *J. Chem. Phys.* 112, 8038-8042 (2000).

C_2H_2+hν
Rydberg State
Predissociative
Lifetimes
Pump/Probe Method

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IR MPD
C_2H_3Br/Ar
C_2,CH,LIF
C_2H_2,HBr,H_2
Products

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C_2F_5COF+hν
C_2F_5COCl+hν
Products
Quantum Yields
Mechanisms

85650. Furlan, A., H.A. Scheld and J.R. Huber, "The Two Competitive Photodissociation Channels in Cyano Carbonyls (NCC(O)X,X=CH_3, $CH(CH_3)_2$, $C(CH_3)_3$, OCH_3) at 193 nm: A Study by Photofragment Translational Energy Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1920-1929 (2000).
RCOCN+hν
R-CH_3,CH_3O,
i-C_3H_7,*t*-C_4H_9
Major Channels

85651. Harich, S., J.J. Lin, Y.T. Lee and X. Yang, "Photodissociation Dynamics of Propyne at 157 nm," *J. Chem. Phys.* 112, 6656-6665 (2000).
C_3H_4+hν
D-Labeling
Fragment Energies
Dynamics

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$C_3H_5I(6\nu_{CH})$+hν
Dissociation
Rate Constants
RRKM Analysis

85653. Wu, S.M., J.J. Lin, Y.T. Lee and X. Yang, "Site Specific Dissociation Dynamics of Propane at 157 nm Excitation," *J. Chem. Phys.* 112, 8027-8037 (2000).
C_3H_8+hν
CH_3,H,H_2
Product Energies
D-Labeling
Branching Ratios

85654. Sevy, E.T., M.A. Muyskens, S.M. Rubin, G.W. Flynn and J.T. Muckerman, "Competition between Photochemistry and Energy Transfer in Ultraviolet-Excited Diazabenzenes. I. Photofragmentation Studies of Pyrazine at 248 nm and 266 nm," *J. Chem. Phys.* 112, 5829-5843 (2000).
c-$C_4H_4N_2$+hν
HCN Quantum Yields
Multiphoton Effects
Rate Constant Measurements

(85376) Aerosol Formation, FTIR Product Analysis
$C_{10}H_8/O_2$+hν

(85837) Fragmentation Spectra, Jet Cooled, Threshold Measurements, D_0 Values
Fe^+CH_2,Co^+CH_2+hν
Ni^+CH_2+hν

85655. Trushin, S.A., W. Fuss, K.L. Kompa and W.E. Schmid, "Femtosecond Dynamics of $Fe(CO)_5$ Photodissociation at 267 nm Studied by Transient Ionization," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1997-2006 (2000).
$Fe(CO)_5$+hν
Product Formation
fs Probe
5 Consecutive Channels

85656. Mahmood, Z., I. Hussain, R.E. Linney and D.K. Russell, "Comparative Infrared Laser Powered Homogeneous Pyrolysis Studies of Triethylgallane, Trimethylgallane, Triisopropylgallane, Triisobutylgallane and Tri-*tert*-Butylgallane," *J. Anal. Appl. Pyrolysis* 44, 29-48 (1997).
IR MPD
$Ga(CH_3)_3$,$Ga(C_2H_5)_3$
$Ga(C_3H_7)_3$,$Ga(C_4H_9)_3$
Products
Comparisons

85657. Fang, W.-H., "Photodissociation of HN_3 at 248 nm and Longer Wavelength: A CASSCF Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 4045-4050 (2000).
HN_3+hν
Channels
Photodissociation
Dynamics

85658. van Harrevelt, R., and M.C. van Hemert, "Photodissociation of Water. II. Wavepacket Calculations for the Photofragmentation of H_2O and D_2O in the B-Band," *J. Chem. Phys.* 112, 5787-5808 (2000).
$H_2O,D_2O+h\nu$
OH/OD(A/X) Branching Ratios
v,J Distributions
Calculations

85659. Votava, O., D.F. Plusquellic, T.L. Myers and D.J. Nesbitt, "Bond-Breaking in Quantum State Selected Clusters: Inelastic and Nonadiabatic Intracluster Collision Dynamics in $Ar(H_2O) \rightarrow Ar+H(^2S)+OH(^2\Pi_{1/2,3/2}{}^{\pm};N)$," *J. Chem. Phys.* 112, 7449-7460 (2000).
$H_2O(3\nu_{OH})+h\nu$
$H_2O.Ar(3\nu_{OH})+h\nu$
Product OH Distributions
Cluster Effects

(85740) Driving Photolysis for a $Br(^2P_{1/2})/CO_2$ Pumped Chemical Laser
$IBr+h\nu$

85660. Nakai, Y., T. Wakabayashi and Y. Ishikawa, "Neutral Molybdenum Atom and Dimer Formations in Laser Induced Plasma: Emission Study of 355 nm Pulse Laser Photolysis of $Mo(CO)_6$ in the Gas Phase," *Appl. Phys. B. Laser Opt.* 66, 621-631 (1998).
UV MPD
$Mo(CO)_6$
Mo^*,Mo_2^*
Product Emissions

85661. Manaa, M.R., "Photodissociation of NaK: Ab Initio Spin-Orbit Interactions of the $Na(3^2S)$ $K(4^2P_J)$ Manifold," *Int. J. Quantum Chem.* 75, 693-697 (1999).
$NaK+h\nu$
Photodissociation Dynamics
Branching Channels

85662. Bakker, B.L.G., D.H. Parker, P.C. Samartzis and T.N. Kitsopoulos, "Nonresonant Photofragmentation/Ionization Dynamics of O_2 Using Picosecond and Femtosecond Laser Pulses at 248 nm," *J. Chem. Phys.* 112, 5654-5659 (2000).
MPD,MPI
O_2
ps,fs Lasers
Fragmentation
Atoms,Ions

85663. Bakker, B.L.G., and D.H. Parker, "Photophysics of O_2 Excited by Tunable Laser Radiation around 193 nm," *J. Chem. Phys.* 112, 4037-4044 (2000).
$O_2+h\nu$(193 nm)
O^+,O Products
Multiphoton Effects
Mechanisms

85664. Parlant, G., "Classical Survival Probability for Ozone Photodissociation in the Hartley Band," *J. Chem. Phys.* 112, 6956-6958 (2000).
$O_3+h\nu$
(D-X) Hartley Band Absorption
Survival Probability
Theory

85665. Makarov, G.N., E. Ronander, S.P. van Heerden, M. Gouws and K. van der Merwe, "Infrared Multiphoton Absorption of SF_6 in Flow with Ar at Moderate Energy Fluences," *Appl. Phys. B. Laser Opt.* 65, 583-587 (1997).
IR MPA
SF_6/Ar
Laser Fluence Dependences

(85377) Particle Formation, SiTMP=Trimethyl(2-propynyloxy) Silane, Laser Induced Nucleation
SiTMP/$C_5H_8+h\nu$

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions)

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85667.	Pisano, P.J., and J.I. Cline, "Determination of μ-v-j Vector Correlations in the Photodissociation Experiments Using (2+n) Resonance-Enhanced Multiphoton Ionization with Time-of-Flight Mass Spectrometer Detection," *J. Chem. Phys.* 112, 6190-6200 (2000).	CH_3 Photofragment Correlations (2+n) REMPI Probe $CH_3I+h\nu$ (2+1) REMPI CH_3 Testing
85668.	He, G., I. Tokue and R.G. Macdonald, "Rotational and Translational Energy Distributions of CN(v=0,J) from the Hot Atom Reactions: $H+XCN \rightarrow HX+CN(v=0,J)$, where X=Br, Cl and CN," *J. Chem. Phys.* 112, 6689-6699 (2000).	CN(v=0,J) Product Distribution 'Hot' H+XCN X=Br,Cl,CN Reaction Cross Sections
85669.	Coronado, E.A., V.S. Batista and W.H. Miller, "Nonadiabatic Photodissociation Dynamics of ICN in the A-Continuum: A Semiclassical Initial Value Representation Study," *J. Chem. Phys.* 112, 5566-5575 (2000).	$CN(J),I(^2P_{1/2,3/2})$ Product Distributions $ICN+h\nu$ Calculations
85670.	Sugita, A., M. Mashino, M. Kawasaki, Y. Matsumi, R. Bersohn, G. Trott-Kriegeskorte and K.-H. Gericke, "Effect of Molecular Bending on the Photodissociation of OCS," *J. Chem. Phys.* 112, 7095-7101 (2000).	CO(v=0,J) Product Distributions $OCS(v=0,1)+h\nu$ $OCS^*+2h\nu$ Mechanisms
85671.	McGivern, W.S., O. Sorkhabi, A.H. Rizvi, A.G. Suits and S.W. North, "Photofragment Translational Spectroscopy with State-Selective 'Universal Detection': The Ultraviolet Photodissociation of CS_2," *J. Chem. Phys.* 112, 5301-5307 (2000).	$CS,S(^1D,^3P)$ Product Energy Distributions $CS_2+h\nu$ Branching Ratio Measurements
(85497)	Product Energy Dependences, $Ca(^1D)+HBr$, Cross Sections, Dynamics	CaBr(B,A)

85672. Delmdahl, R.F., B.L.G. Bakker and D.H. Parker, "Completely Inverted ClO Vibrational Distribution from $OClO(^2A_2,24,0,0)$," *J. Chem. Phys.* 112, 5298-5300 (2000).

$ClO(v),O(^3P_2)$
Product Energies
$ClO_2+h\nu$
Dynamics

85673. Zhang, L., M.-D. Chen, M.-L. Wang and K.-L. Han, "Product Rotational Polarization: Stereodynamics of the Reaction $Cl(^2P_{3/2})+CD_4(v=0,j=0)\rightarrow DCl(v'=0,j'=1)+CD_3$," *J. Chem. Phys.* 112, 3710-3716 (2000).

$DCl(v=0,J=1),CD_3$
Product Angular
Rotational
Polarization
$Cl+CD_4$
Calculations

85674. Truhins, K., R. Marsh, A.J. McCaffery and T.W.J. Whiteley, "A Simple Model for Product Rovibrational Distributions in Elementary Chemical Reactions," *J. Chem. Phys.* 112, 5281-5291 (2000).

HCl,HF,HD
v,J Product
Distributions
$Cl+H_2$
$F+I_2$
$H+D_2$
Simple Model

85675. Liu, D.-K., and K.-C. Lin, "Nascent Rotational Distributions of MgH in Reaction of $Mg(4s^1S_0)$ with H_2 and HD," *J. Chinese Chem. Soc.* 44, 463-468 (1997).

MgH(v=0,1,J)
Product
Distributions
$Mg(^1S_0)+H_2$,HD
Mechanism

85676. Chiang, S.-Y., and C.-I. Ma, "Fragmentation of Vibrationally Selected N_2O^+ in State $C^2\Sigma^+$ from Measurements of Threshold Photoelectron Photoion Coincidence," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1991-1996 (2000).

N^+,O^+
NO^+,N_2^+
Fragment Energies
$N_2O^+(C,v)$
Dissociation
Dynamics

85677. Umemoto, H., N. Terada and K. Tanaka, "Verification of the Insertion Mechanism of $N(2^2D)$ into H-H Bonds by the Vibrational State Distribution Measurement of $NH(X^3\Sigma^-,0\leq v\leq 3)$," *J. Chem. Phys.* 112, 5762-5766 (2000).

$NH(X,v\leq 3)$
Product
Distribution
$N(^2D)+H_2$
Mechanism

85678. Reid, J.P., R.A. Loomis and S.R. Leone, "Characterization of Dynamical Product-State Distributions by Spectral Extended Cross Correlation: Vibrational Dynamics in the Photofragmentation of NH_2D and ND_2H," *J. Chem. Phys.* 112, 3181-3191 (2000).

NH_2,NHD,ND_2(A)
Product FTIR
Spectral Emission
$NH_3,ND_3+h\nu$
$NH_2D,ND_2H+h\nu$
Branching Ratios

85679. Monti, O.L.A., H. Dickinson, S.R. Mackenzie and T.P. Softley, "Rapidly Fluctuating Anisotropy Parameter in the Near-Threshold Photodissociation of NO_2," *J. Chem. Phys.* 112, 3699-3709 (2000).

$NO(J=17/2),O(^3P_2)$
Product
Anisotropy
$NO_2+h\nu$
Near Threshold
State Selective
Excitation

85680. Brouard, M., D.W. Hughes, K.S. Kalogerakis and J.P. Simons, "The Product Rovibrational and Spin-Orbit State Dependent Dynamics of the Complex Reaction $H+CO_2 \rightarrow OH(^2\Pi;v,N,\Omega,f)+CO$: Memories of a Lifetime," *J. Chem. Phys.* 112, 4557-4571 (2000).

$OH(v,N,\Omega,f)$
Product
Distributions
'Hot' $H+CO_2$
Cross Sections
Collision Dynamics

85681. Shin, S.K., E.J. Han and H.L. Kim, "Photodissociation Dynamics of Formic Acid at 193 nm," *J. Photochem. Photobiol. A. Chem.* 118, 71-74 (1998).

OH(v,J)
Product Energies
$HCOOH+h\nu$

85682. Zanganeh, A.H., J.H. Fillion, J. Ruiz, M. Castillejo, J.L. Lemaire, N. Shafizadeh and F. Rostas, "Photodissociation of H_2O and D_2O below 132 nm," *J. Chem. Phys.* 112, 5660-5671 (2000).

OH/OD(A,v,J)
Fragment Energies
$H_2O/D_2O+h\nu$
Mechanism

85683. Ramachandran, B., "Energy Disposal in the $O(^3P)+HCl$ Reaction: Classical Dynamics and Comparison to Experiment," *J. Chem. Phys.* 112, 3680-3688 (2000).

OH(v,J)
Product Energy
Distributions
$O+HCl(v=2,J=1,6,9)$
Calculations

(85522) $O(^1D)+SiH_4$, Reaction Dynamics, Calculations

SiO
Product Energies

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

85684. Longevialle, P., O. Lefevre, N. Mollova and G. Bouchoux, "Further Arguments Concerning a 'Rotational Effect' in the Unimolecular Fragmentations of Organic Ions in the Gas Phase," *Rapid Commun. Mass Spectrom.* 12, 57-60 (1998).

Unimolecular
Fragmentation
Organic Ions
Rotational
Effects

85685. Wang, B., H. Hou and Y. Gu, "A Theoretical Study of the Thermal Decomposition of Fluoromethanethiol, CH_2FSH," *Phys. Chem. Chem. Phys.* 1, 4733-4738 (1999).

Unimolecular
Dissociation
CH_2FSH
Product Channels
Species ΔH_f
Calculations

(85780) Isomerizations, Isomers, Structural Calculations, Geometries, ΔH_f — C_2H_3S, $C_2H_3S^+$

85686. King, R.A., W.D. Allen and H.F. Schaefer III, "On Apparent Quantized Transition State Thresholds in the Photofragmentation of Acetaldehyde," *J. Chem. Phys.* 112, 5585-5592 (2000). — Unimolecular Dissociation, $CH_3CHO(T_1)$, RRKM Analysis, Difficulties

85687. Tanaka, C., and J. Tanaka, "Ab Initio Molecular Orbital Studies on the Chemiluminescence of 1,2-Dioxetanes," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2078-2090 (2000). — Unimolecular Dissociation, $C_2H_4O_2$, $C_2(CH_3)_4O_2$, Product Chemiluminescence Channels

85688. Moskaleva, L.V., L.K. Madden and M.C. Lin, "Unimolecular Isomerization/Decomposition of *ortho*-Benzyne: ab Initio MO/Statistical Theory Study," *Phys. Chem. Chem. Phys.* 1, 3967-3972 (1999). — Unimolecular Isomerization, *o*-C_6H_4, Dissociation, Rate Constants, Calculations

85689. Takahashi, Y., T. Higuchi, O. Sekiguchi, M. Ubukata and S. Tajima, "Unimolecular Hydrogen Chloride Loss from the Molecular Ions of Chlorophenols: A 'Ring-Walk' Mechanism for a Chlorine Ion," *Rapid Commun. Mass Spectrom.* 13, 393-397 (1999). — Unimolecular Dissociation, $C_6H_4(Cl)OH^+$, HCl Loss Channel, Mechanism

85690. Fadden, M.J., C. Barckholtz and C.M. Hadad, "Computational Study of the Unimolecular Dissociation Pathways of Phenylperoxy Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3004-3011 (2000). — Unimolecular Dissociation, $C_6H_5O_2$, P.E. Surface, Channels

85691. Cattaneo, P., and M. Persico, "An ab Initio Study of the Photochemistry of Azobenzene," *Phys. Chem. Chem. Phys.* 1, 4739-4743 (1999). — Isomerization, $C_6H_5NNC_6H_5$, Photoinduced Dynamics

85692. Warmuth, C., F. Milota, H.F. Kauffmann, H. Wadi and E. Pollak, "Experimental Evidence of Laser Cooling of Room Temperature *trans*-Stilbene upon Excitation to the S_1 State," *J. Chem. Phys.* 112, 3938-3941 (2000). — Isomerization, $(C_6H_5CH)_2$, S_1, Photoinduced, Fluorescence, Lifetimes

(85785) Isomerization, IR, Raman Spectra, D-Substitutions, Structural Calculations, Geometries, Frequencies — *cis-,trans*$(C_6H_5CH)_2$

(85123) Unimolecular Dissociation Channels, Energies — RDX

85693. Christoffel, K.M., and J.M. Bowman, "Quantum Scattering Calculations of Energy Transfer and Isomerization of HCN/HNC in Collisions with Ar," *J. Chem. Phys.* 112, 4496-4505 (2000).

Isomerization
HCN/HNC+Ar
Reaction Dynamics
Energy Transfer
Calculations

85694. Joyeux, M., D. Sugny, V. Tyng, M.E. Kellman, H. Ishikawa, R.W. Field, C. Beck and R. Schinke, "Semiclassical Study of the Isomerization States of HCP," *J. Chem. Phys.* 112, 4162-4172 (2000).

Isomerization
HCP
Vibrational
Energy Levels
P.E. Surface
Calculations

85695. Yamamoto, T., and S. Kato, "Full-Dimensional Quantum Dynamics Study on the Mode-Specific Unimolecular Dissociation Reaction of HFCO," *J. Chem. Phys.* 112, 8006-8016 (2000).

Unimolecular
Dissociation
HFCO
Rates
Mode Dependences
Calculations

(85793) Isomerization, Geometries, Frequencies, Structural Calculations

$(NO)_2$

85696. Wang, X., and Q.-Z. Qin, "Photoisomerization of N_2O_3 in an Ar Matrix," *J. Photochem. Photobiol. A. Chem.* 122, 1-5 (1999).

Isomerization
N_2O_3
Photon Induced
FTIR Spectra
Matrix Study

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

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Reaction Dynamics
A+BC
Rates,VTST
Calculation Code

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Reaction Dynamics
Br+HO_2
BrO+OH
[$HBrO_2$] Isomers
P.E. Surfaces
Channels

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Reaction Dynamics
CH+N_2
Spin-Forbidden
Channel
P.E. Surfaces

85700. Okamoto, Y., and M. Tomonari, "Ab Initio Calculations on Reactions of CHF_3 with Its Fragments," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2729-2733 (2000).

Reaction Dynamics
CHF_3+X
$X=CHF_3, CF_3, CF_2, CHF_2, CHF, CF, CH, F, H$
Channels

85701. Collins, M.A., S. Petrie, A.J. Chalk and L. Radom, "Proton-Transport Catalysis and Proton-Abstraction Reactions: An ab Initio Dynamical Study of $X+HOC^+$ and XH^++CO($X=$Ne, Ar and Kr)," *J. Chem. Phys.* 112, 6625-6634 (2000).

Reaction Dynamics
COH^++Rg
RgH^++CO
P.E. Surfaces
Channels

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$CH_2Br+HBr$
Channels
Energy Barriers
Transition States

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CH_2Br_2+OH
Rate Constants
Screening Tool
Method

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CH_3+CH_3+M
Rate Constants
VTST
Calculations

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CH_4+OH
P.E. Surface
D-Isotopes
Accuracies

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$C_2H_2+H_2O$
P.E. Surface
Structures

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C_2H_3+NO
P.E. Surface
Channels

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$CH_2CHOH^+/CH_3CHO^+/CH_3COH^+$
P.E. Curves
Isomerization
Energies
$\Delta H_f(CH_3COH^+)$

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ROOH Radicals
OH Loss Channel
Cyclic Ether Product
Rate Constants

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$C_4H_8+O_3$
Isomeric Effects
Channels

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$C_{60}+O_3$
Mechanism

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Reaction Dynamics
ClO+OH
P.E. Surfaces
HCl Product Channel

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$Co^+ + C_3H_8$
P.E. Surface
Channels
Energies

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$Cs+H_2$
$Ti+O_2$
Laser Monitoring Techniques
Product Channels

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$F+H_2$
Cross Sections
Surface Comparisons

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Reaction Dynamics
$H+D_2(v,J)$
Probabilities
Geometric
Phase Effects

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Reaction Dynamics
$H+H_2$
QTST
Rate Constants

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$H+H_2S$
Rate Constants
Erratum

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$H^+ + O_3$
P.E. Surface
Conical
Intersections

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H_2+He
Dissociation
Cross Sections
Fragment Energies

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NH_2+NO
Channels
Rate Constants
Branching Ratio

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$O+HO_2$
P.E. Surface
Rate Constant
Mechanism

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$OH+H_2$
Rate Constants
Energy Barrier
Calculations

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$O_2^- + O_2$
Electron Transfer
Reactivity

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Reaction Dynamics
$Ti^+ + CH_4$,HF,HCl
$Ti^+ + H_2O, H_2S$
$Ti^+ + NH_3, PH_3, SiH_4$
Insertion
Excited State Effects

41. CHEMICAL KINETICS - GENERAL

(85112) Solid Propellant, Acoustic Induced, Modeling

Flame Oscillations

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CH_4, C_2H_2, C_2H_4
RF Discharges
Powder Formation
Absorption/
Mass Analysis

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$(CH_3)_2S/O_2/OH$
Product FTIR
Analysis
T,O_2 Dependences
Mechanism

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$C_6H_5 + CH_3CCH$
Crossed Beam
Reaction Dynamics
H Atom Loss
Channel

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$C_6H_{6-n}(CH_3)_n + O$
n=1-3
Ar Matrix Study
Products
D-Labeling

(85509) Cross Beam Interactions, Products

$Mo + CH_4, C_2H_6$

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NH+NO
HNNO Intermediate
FTIR Spectrum
Matrix Study

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N_2
Microwave Discharge
Afterglows
$N_2(B), N_2^+(B)$
Species Histories

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N_2/O_2
Pulsed Discharge
$NO(B,A),N_2(B,C)$
Afterglow
Kinetics

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N_2O
Hollow Cathode Discharge
Kinetic Modeling
Transient Profiles

(85242) Catalytic Induced Oscillations, Kinetic Model

N_2O
Dissociation

(85825) BrO_2 Product, Formation Mechanism

$O+Br_2$

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$OH(v)+H_2(v')$
$\nu_{OH}=2,\nu_{H2}=1$
Collision Complex
Predissociation
Dynamics
Lifetimes

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$OH+NO_2+M$
$HONO_2$,HOONO
Product Channels
Calculations

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O_3 Formation
Air Discharge
Kinetic Model

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SiF_2+SiF_4
Lewis Base
Induced Reaction

42. LASERS/INDUCED EFFECTS/MPI

(See also Section 26 for REMPI Spectra)

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Laser Crystal
Diode Pumped
Performance
Comparisons

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(85388)	Mass Analysis, Aerosol Particle Analysis Method	Laser Ablation/ Ionization
85741.	Hermann, J., and C. Dutouquet, "Analyses of Gas Phase Reactions during Reactive Laser Ablation Using Emission Spectroscopy," *J. Phys. D. Appl. Phys.* 32, 2707-2713 (1999).	Laser Ablation Al,C,Ti/N_2,O_2 Emission Spectra Plume Chemistry
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(85586)	Sooting Flame, C_2(e-a,D-B′) LIF, Laser Vaporization Formation	Laser Ablation Soot
85743.	Man, B.Y., "Particle Velocity, Electron Temperature, and Density Profiles of Pulsed Laser Induced Plasmas in Air at Different Ambient Pressures," *Appl. Phys. B. Laser Opt.* 67, 241-245 (1998).	Laser Ablation Ti Alloys Fe*,Ti* Emission Velocities Temperatures
(85847)	Axis Alignment Determination, (1+1)/Photoelectron Distribution Procedure	REMPI
(85549)	Ultrasensitive Detection System	2-Color REMPI/ Ion Cloud Chamber
85744.	Mathur, D., and K. Vijayalakshmi, "Angle-Resolved Mass Spectrometry of Chloromethanes in an Intense Laser Field," *Rapid Commun. Mass Spectrom.* 12, 246-250 (1998).	MPI CCl_4,$CHCl_3$ CH_2Cl_2 Fragmentations Polarization Effects
(85667)	(2+1) Mode, Photolysis Photofragmentation Correlation Testing, CH_3I+hν	CH_3,REMPI

(85200) Product Velocity Mapping, $CH_3I + h\nu$ — $CH_3(v), I(^2P_{1/2,3/2})$ REMPI

(85550) REMPI/TOF Mass Spectrum, Surrogate Monitor for Flue Gas PCDD/PCDFs — C_6H_5Cl, REMPI

(85306) Rich Flames, Formation Monitoring — PAH, Fullerenes REMPI

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(85662) Nonresonant Fragmentation, Atoms, Ions, ps, fs Lasers, Measurements — O_2, MPI

(85663) 193 nm ArF Laser, Multiphoton Absorption, Mechanisms — O_2, MPI

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects and Section 40 for Surface Dynamics)

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Vibrational
Energy Levels
$Na_3(1^4A_2')$
Calculations

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Diatomics
Universal
Expressions

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Analytical
Potential Form
Diatomics
H_2,N_2,O_2
Electronic States

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Global Fitting
Computer Code

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P.E. Surfaces
$Al(^2P)/H_2$
$B(^2P)/H_2$
van der Waals
Complexes
Well Depths

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P.E. Curves
AlS,$AlS^{\pm}$
Low-lying States
Spectral Constants
Transition Moments
B-State Lifetime

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ArO,ArO^-
Ion PES Spectrum
Well Depths
States

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$B_2H_2(1^1\Delta_g)$
Vibronic Spectrum
Calculations

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P.E. Curves
Be_2
Low-lying States
Spectral Constants
D_e

(85210) P.E. Curve, Ion Mobility Calculations — CO^+/He

(85690) P.E. Surface, Unimolecular Dissociation, Channels — $C_6H_5O_2$

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HBr,DBr(E)
E/V Interaction
Tunneling
Measurements

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P.E. Surfaces
HCP
Low-lying States
Energy Levels
Calculations

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P.E. Surfaces
H_2O
9 Low-lying States
Avoided Crossings
Conical Intersection

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P.E. Surfaces
H_2+O
Lowest $^3A',^3A''$
Calculations

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P.E. Curves
IO
Low-lying States
Spectral Constants
D_0
Calculations

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P.E. Curve
$K_2(2^1\Sigma_g^+)$
LIF Spectra
Constants

(85508) P.E. Curves, (F,E) Calculations, F-State RKR Measurements — Li_2(F,E)

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P.E. Surface
NH_2(A)
$N(^2D)+H_2$
NH(a)+H
Correlations
Energies

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P.E. Curves
NaK(c,b,a)
LIF Spectra
Dunham Constants

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P.E. Curves
NaO^+(d,c,b,a,A,X)
NaO(A,X)
Spectral Constants
D_e,F.C. Factors
Calculations

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P.E. Curves
Na_2(a,X)
Construction
Method
Accuracies

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P.E. Curve
$Na_2(4^3\Sigma_g^+)$
Vibrational
Levels
Constants
OODR Spectra

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P.E. Curves
O_3
Low-lying
Singlet States
Construction

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PO(X)
Spectral Constants
v,J Energy Levels
Lifetimes
Calculations

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RgX_2
Status
Review

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P.E. Curves
WC
Low-lying States
Spectral Constants
D_0

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(See also Section 26 for Spectrally Measured Structures)

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85779.	Stanton, J.F., "A Refined Estimate of the Bond Length of Methane," *Mol. Phys.* 97, 841-845 (1999).	Structural Calculations CH_4 Geometry r_e
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Structural Calculations
$CH_3C(O)OO$
$CH_3C(O)OONO_2$
Geometries
Frequencies
IR Intensities
D_0

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Structural Calculations
$C_2O(A,X)$
Geometries
Frequencies
IR Intensities

(85831) Structural Calculations, Geometries, Frequencies, ΔH_f

C_3H_4 ,C_3H_5
c-C_3H_4 ,*c*-C_3H_6
C_3H_6 ,C_3H_8

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$C_4H_6(2^1A_g ,1^1B_u)$
Excitation Energies
Geometries

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Structural Calculations
C_6H_6
Equilibrium Geometry

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Structural Calculations
cis-,trans$(C_6H_5CH)_2$
Geometries
Frequencies
Isomerization
IR,Raman Spectra
D-Substitutions

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Structural Calculations
Cl_2O_n ,$Cl_2O_n^+$
n=1-7
Geometries
Energies

(85215) Isomeric Ions, Formation, Structure, Calculations

$Cl_2O_2^+$,$Cl_2O_2^-$

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Structural Calculations
CuH,CuCl,Cu_2
AgH,AgCl,Ag_2
AuH,AuCl,Au_2
Geometries
Frequencies
D_0 ,Dipole Moments

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Structural Calculations
FO_2 ,ClO_2 ,BrO_2
$FO_2^{\pm}$,$ClO_2^{\pm}$,$BrO_2^{\pm}$
ClO_3
Geometries
Frequencies
D,IP,EA

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Structural Calculations
(GeCH),$(GeCH)^+$
Isomers
Geometries
Energies

(85828) Structural Calculations, P.E. Surfaces, Geometries, Frequencies, D_0 , IP, EA

HCO,$HCO^{\pm}$

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HO_2+RCHO,$(CH_3)_2CO$
OH+RCHO,$(CH_3)_2CO$
R=H,CH_3
Addition Complex Stabilities

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Structural Calculations
H_2^+,HD^+,D_2^+
Bond Lengths
Vibrational Dependence

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Structural Calculations
$Li(H_2O)_n$
$Na(H_2O)_n$
Geometries
Frequencies

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(85748)	Structural Calculations, Geometry, Frequencies, v,J Energy Levels	OCSe
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85798.	Demaison, J., L. Margules, J. Breidung, W. Thiel and H Burger, "Ab Initio Anharmonic Force Field, Spectroscopic Parameters and Equilibrium Structure of Trifluorosilane," *Mol. Phys.* 97, 1053-1067 (1999).	Structural Calculations $SiHF_3$ Geometry Spectral Constants
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(85844)	Structural Calculations, Force Field, ΔH_f	SiH_4

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Structural Calculations XeO_2 ,XeO_3 XeO_4 Geometries Frequencies

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(See also Section 27 for Electronically Excited State Relaxation Processes)

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Rotational Relaxation
$CH_4(J)+Ar$
Diode Laser Spectra
Rates

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Rotational Relaxation
CN(A,v=3,N=60)
Ar Collisions
Rate Constants
Propensities

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Rotational
S/O Energy Transfer
$NO(X^2\Pi)+Ar$
Cross Sections
Calculations

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Equilibrium Composition
Calculations
Method

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Equilibrium Compositions
Thermodynamic Error Influence
Assessment

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Vapor Pressure
Measuring Methods
Thermodynamic Data Source
Overview

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D_0
30 Molecules
DFT Method
Accuracies

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ΔH_f
Large Data Set
G-3 Testing
Adequacies

(85434) Anion Photoelectron Spectra, Frequencies, Structures

EA(AgCN,CuCN)

(85787)	D_0, Dipole Moments, Geometries, Frequencies, Structural Calculations	AgH,AgCl,Ag_2 AuH,AuCl,Au_2 CuH,CuCl,Cu_2
(85755)	P.E. Surfaces, Well Depths, van der Waals Complexes	$Al(^2P)/H_2$ $B(^2P)/H_2$
(85757)	P.E. Curves, Well Depths, Ion Photoelectron Spectrum, Electronic States	ArO,ArO^-
(85777)	D_e, Structures, Spectral Constants, Calculations	BH,BH^+,CH,$CH^\pm$ NH,$NH^\pm$,OH(A,X) OH^+,HF,HF^+
(85408)	Ba, Ba^+ Emission Spectra, Energy Levels	IP(Ba)
85824.	Boutou, V., M.A. Lebeault, A.R. Allouche, F. Paulig, J. Viallon, C. Bordas and J. Chevaleyre, "Electronic Properties of Mixed Barium-Oxygen Clusters," *J. Chem. Phys.* 112, 6228-6236 (2000).	IP(Ba_nO_m) n=2-13,m≤n Measurements
(85759)	P.E. Curves, Low-lying States, Spectral Constants, Calculations	$D_e(Be_2)$
85825.	Dyke, J.M., S.D. Gamblin, N. Hooper, E.P.F. Lee, A. Morris, D.K.W. Mok and F.T. Chau, "A Study of the BrO and BrO_2 Radicals with Vacuum Ultraviolet Photoelectron Spectroscopy," *J. Chem. Phys.* 112, 6262-6274 (2000).	IP(BrO),D(BrO^+) IP(BrO_2) PES Spectra O+Br_2 BrO_2 Product Mechanism
85826.	Barden, C.J., and H.F. Schaefer III, "The Singlet-Triplet Separation in Dichlorocarbene: A Surprising Difference between Theory and Experiment," *J. Chem. Phys.* 112, 6515-6516 (2000).	$^{1,3}CCl_2$ Energy Separation Calculations
85827.	Bauschlicher Jr., C.W., "The Scalar Relativistic Contribution to the Atomization Energies of CF, CF_4 and SiF_4," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2281-2283 (2000).	Atomization Energies CF,CF_4 SiF_4 Calculations
(85685)	Thirteen Sulfur Species, CH_2FSH Unimolecular Dissociation Involvement, Calculations	ΔH_f (C/H/F/S)
85828.	van Mourik, T., T.H. Dunning Jr., and K.A. Peterson, "Ab Initio Characterization of the HCO^x(x=-1,0,+1) Species: Structures, Vibrational Frequencies, CH Bond Dissociation Energies and HCO Ionization Potential and Electron Affinity," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2287-2293 (2000).	D_0,IP,EA(HCO) P.E. Surfaces Geometries Frequencies Calculations
85829.	Jarvis, G.K., K.-M. Weitzel, M. Malow, T. Baer, Y. Song and C.Y. Ng, "High Resolution Pulsed Field Ionization Photoelectron-Photoion Coincidence Study of C_2H_2: Accurate 0 K Dissociation Threshold for C_2H^+," *Phys. Chem. Chem. Phys.* 1, 5259-5262 (1999).	IP(C_2H) $\Delta H_f(C_2H^+)$ PFI-PEPICO Measurements
(85495)	(B-X) Fluorescence, Predissociative Lifetimes	D_0(CCH)

85830.	Le, H.T., M. Flock and M.T. Nguyen, "On the Triplet-Singlet Energy Gap of Acetylene," *J. Chem. Phys.* 112, 7008-7010 (2000).	Energy Splitting $C_2H_2(^3B_2/X)$ Calculations
(85708)	P.E. Curves, Isomerizations, Calculations	$\Delta H_f(CH_3COH^+)$
(85781)	Structural Calculations, Geometries, Frequencies, IR Intensities	$D(CH_3C(O)OO)$ $D(CH_3C(O)OONO_2)$
(85780)	Isomers, Geometries, Isomerizations, Structural Calculations	$\Delta H_f(C_2H_3S)$ $\Delta H_f(C_2H_3S^+)$
(85424)	2-Photon PFI-PE Spectra, A/X Energy Separation	IP(C_2H_5S(A,X))
85831.	Feller, D., and D.A. Dixon, "Predicting the Heats of Formation of Model Hydrocarbons up to Benzene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3048-3056 (2000).	ΔH_f C_3H_4 ,C_3H_5 *c*-C_3H_4 ,C_3H_6 ,C_3H_8 *c*-C_3H_6 Geometries Frequencies Calculations
(85618)	C_3H_5+HBr Rate Constant Measurements, Equilibrium Constant Analysis	$\Delta H_f(C_3H_{5)}$
85832.	Baer, T., Y. Song, C.Y. Ng, J. Liu and W. Chen, "The Heat of Formation of 2-$C_3H_7^+$ and Proton Affinity of C_3H_6 Determined by Pulsed Field Ionization-Photoelectron Photoion Coincidence Spectroscopy," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1959-1964 (2000).	ΔH_f(2-$C_3H_7^+$) Pulsed Field Ionization Measurement
85833.	Rienstra-Kiracofe, J.C., G.B. Ellison, B.C. Hoffman and H.F. Schaefer III, "The Electron Affinities of C_3O and C_4O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2273-2280 (2000).	EA(C_3O) EA(C_4O) Calculations
(85430)	Photodissociation Spectra, Constants	$D_0(Ca^+.Ne(D,C,X))$
85834.	Rau, J.V., N.S. Chilingarov and L.N. Sidorov, "Mass Spectrometric Determination of Cobalt Trifluoride Saturated Vapor Pressure: Enthalpy of Formation of Gaseous CoF_4 and CoF_4^-," *Rapid Commun. Mass Spectrom.* 11, 1977-1979 (1997).	$\Delta H_f(CoF_3, CoF_4)$ EA(CoF_4) Knudsen Cell Measurements
(85433)	Low-lying Electronic States, Spectral Constants, T_e, Calculations	D_e(CrF,CrCl)
85835.	Sarkisyan, D.H., A.S. Sarkisyan and A.K. Yalanusyan, "Thermal Dissociation of Cesium Dimers," *Appl. Phys. B. Laser Opt.* 66, 241-244 (1998).	$D(Cs_2)$ Thermal Dissociation Dimer Density Sealed Cell Measurement Method

85836.	Ingolfsson, O., U. Busolt and K.-i. Sugawara, "Energy-Resolved Collision-Induced Dissociation of Cu_n^+ (n=2-9): Stability and Fragmentation Pathways," *J. Chem. Phys.* 112, 4613-4620 (2000).	$D(Cu_n^+)$ n=2-9 Collision Induced Dissociation Measurements
(85788)	Neutral, Anion, Cation Structural Calculations, Geometries, Frequencies	D,IP,EA FO_2,ClO_2 ClO_3,BrO_2
85837.	Husband, J., F. Aguirre, C.J. Thompson, C.M. Laperle and R.B. Metz, "Photofragment Spectroscopy of $FeCH_2^+$, $CoCH_2^+$ and $NiCH_2^+$ Near the M^+-CH_2 Dissociation Threshold," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 2020-2024 (2000).	$D_0(Fe^+CH_2,Co^+CH_2)$ $D_0(Ni^+CH_2)$ Photolysis Threshold Measurements
85838.	Litorja, M., and B. Ruscic, "A Photoionization Study of the Hydroperoxyl Radical, HO_2, and Hydrogen Peroxide, H_2O_2," *J. Electron Spectrosc. Relat. Phenom.* 97, 131-146 (1998).	IP,$\Delta H_f(HO_2)$ IP,$D_0(H_2O_2)$ PA(O_2) Photoionization Measurements
(85454)	2-Photon, 1-Color ZEKE-PFI Spectrum, Neutral/Ion Constants	IP$(IBr(X^2\Pi_{1/2,3/2}))$
(85764)	P.E. Curves, Low-lying States, Spectral Constants, Calculations	$D_0(IO)$
(85456)	(A-X) LIF Spectrum, Ground State Dunham Constants, P.E. Curve	$D_e(KRb)$
85839.	Bencze, L., A. Lesar and A. Popovic, "The Evaporation Thermodynamics of Lithium Iodide: Mass Spectrometric and ab Initio Studies," *Rapid Commun. Mass Spectrom.* 12, 917-930 (1998).	Vaporization LiI(s) $(LiI)_n$ Species Structures Frequencies D_0
(85462)	Ion Photoelectron Spectra, Frequencies, Structures	EA(MC_3) M=Sc thru Ni
(85768)	P.E. Curves, NaO(A,X), NaO^+(d,c,b,a,A,X), Spectral Constants, F.C. Factors, Calculations	$D_e(NaO,NaO^+)$
85840.	Soldan, P., E.P.F. Lee, S.D. Gamblin and T.G. Wright, "Na_2O and Na_2O^+: Thermodynamics and Low-lying Electronic States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 3317-3325 (2000).	$\Delta H_f(Na_2O,Na_2O^+)$ $\Delta H_f(NaO)$ Calculations
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$D_0(SF_6)$
IP(SF_5)
$\Delta H_f(SF_5^+, SF_4^+)$
$\Delta H_f(SF_3, SF_3^+)$
Mass Analysis
$SF_6 + e^-$

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$D_0(SH, SH^-)$
$S^- + H_2, D_2$
Threshold Reaction Energy Measurements

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$\Delta H_f(SiH_4)$
Force Field Calculations

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IP(Si_2)
Photoionization Spectrum
Calculations

(85774) P.E. Curves, Low-lying States, Spectral Constants

D_0(WC)

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D,IP,EA(WF_n)
$n = 1$-6
Calculations

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Axis Alignment Determination
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$Li_2(v = 0, J \geq 115)$
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Above Dissociation Levels

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Electric/Magnetic Field Techniques

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